

# A Particle-Only Hybrid Method For Near-Continuum Flows

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**Abstract.** EPSM is a particle simulation method for the simulation of the Euler equations. EPSM is used here as part of a hybrid EPSM/DSMC method for the simulation of near continuum flows. It is used where the flow gradients are not large and the flow is expected to be in an equilibrium state. The gradient of local mean free path has been used to detect those regions where EPSM can be invoked. Results are presented for the unsteady flow of a gas in a shock tube with Knudsen numbers in the initial state of 0.01 and 0.002 either side of the diaphragm (based on the length of the initial low-pressure region). The results for the hybrid method are very close to those for pure DSMC. The execution speed of the hybrid code is 1.75 times that of standard DSMC.

## 1 INTRODUCTION

DSMC becomes prohibitively computational intensive as it is applied to high-density collision-dominated flows. One way to overcome this is to construct hybrid codes that combine a conventional continuum Navier-Stokes solver and a DSMC code (Wadsworth and Erwin 1990, 1992; Hash and Hassan 1995,1996). The continuum solver is invoked in those (collision-dominated) regions of the flow where the Navier-Stokes equations are valid and DSMC is invoked in those (rarefied) regions of the flow where the Navier-Stokes equations are expected to be invalid.

To save computational effort, Roveda *et al* (1998) have used an Euler solver, rather than a Navier-Stokes solver, for those parts of the flow where DSMC is too computationally expensive. Wherever flow gradients appear in the solution, Euler solvers display numerical dissipation and not the correct Navier-Stokes dissipation. However, provided the Euler solver is invoked in those cells where the flow gradients are small this is not important: the Euler equations are sufficiently accurate outside regions of large flow gradients such as boundary layers and the interior of shocks. DSMC can be used where flow gradients are large and dissipative effects must be accurately modelled.

The chief difficulty with hybrid continuum/DSMC codes lies in the interface between the two approaches. Information from the continuum solver can easily serve as the boundary conditions for DSMC, but it is more difficult to use the “noisy” information from the DSMC solution as boundary conditions for the continuum solution method. This problem seems an inevitable result of the amalgamation of a continuum solver, for which the primitive variables are the continuum flow properties such as density and fluid velocity, and the particle-based DSMC method. However, it would disappear if the continuum regions of the flow could be efficiently calculated with a particle-based method.

I have used Pullin's (1980) particle-based “continuum” method known as EPSM, in a hybrid continuum/DSMC solver. The new hybrid method has been demonstrated using a similar case as Roveda *et al* (1998) - the one-dimensional unsteady shock tube flow. Because particles are used throughout the simulation the interface between the continuum (EPSM) and rarefied (DSMC) regions presents no difficulties; all that changes is the way molecular velocities are established at each time step.

## 2 EQUILIBRIUM PARTICLE SIMULATION METHOD

Pullin (1980) developed a particle simulation method called the Equilibrium Particle Simulation Method (EPSM), as the infinite collision rate or “continuum” limit of DSMC for a given cell network and number of simulator particles. In EPSM, as in DSMC, a flow is simulated by tracking the motion and interactions of a set of representative particles. In EPSM, however, no collisions between particles are calculated, but the effect of collisions is simulated by redistributing the total momentum and energy of all the particles in each cell at each time step amongst all the particles in the cell. That is, new particle velocities, representative of a local Maxwellian equilibrium distribution, are selected at random while preserving the total momentum and energy in each cell. The effect is just as though DSMC were used to calculate an infinite number of collisions amongst the particles in each cell at each time step.

Because the cell sizes and local time step in EPSM will necessarily be larger than the theoretically vanishing mean free path and mean free time in the infinite collision rate limit, EPSM cannot be considered an entirely accurate continuum simulation method wherever there are flow gradients. The dissipation inherent in EPSM (which is approximately the dissipation inherent in DSMC when DSMC is used for high collision rate flows with “large” cell sizes and time steps) is discussed elsewhere (Macrossan 1995). However, in this respect EPSM is similar to any Euler solver.

### 2.1 Velocity selection in EPSM

Here I briefly describe the problem in statistics that arises in EPSM. After the convection stage of the calculation, let the particle velocities in a cell, with components  $u$ ,  $v$  and  $w$ , be  $(u_j, v_j, w_j)$ ,  $j = 1 \dots N$ . Let the required new set of velocities in the cell be  $(u_j^*, v_j^*, w_j^*)$ ,  $j = 1 \dots N$ . The new set of velocity components must be derived from an equilibrium distribution, subject to the constraints that the mean values and the standard deviations of the randomly selected (sample) velocities take specified values. The mean values must be constrained to preserve total momentum,

$$\begin{aligned}\bar{u}_j^* & (= \frac{1}{N} \sum u_j^*) = \bar{u}_j \\ \bar{v}_j^* & (= \frac{1}{N} \sum v_j^*) = \bar{v}_j \\ \bar{w}_j^* & (= \frac{1}{N} \sum w_j^*) = \bar{w}_j\end{aligned}$$

while the variance of each component must be constrained to be equal (the equilibrium constraint) with a value determined by total energy in the cell. Thus, for three degrees of freedom for thermal energy<sup>1</sup>

$$\sum (u_j^* - \bar{u}_j^*)^2 = \sum (v_j^* - \bar{v}_j^*)^2 = \sum (w_j^* - \bar{w}_j^*)^2 = e$$

where

$$e = \frac{1}{3} \left[ \sum (u_j - \bar{u}_j)^2 + \sum (v_j - \bar{v}_j)^2 + \sum (w_j - \bar{w}_j)^2 \right].$$

Pullin (1978) formally derived an algorithm for generating normal variates such that the sample mean and variance were known, while the mean and variance of the normal parent distribution were unknown.

Montanero *et al* (1998), in a slightly different context, were faced with a similar problem: that of selecting a new set of normally distributed velocity components for a set of particles, while preserving total energy and momentum. They did this by a somewhat *ad hoc* procedure whereby velocity components (for the subset of particles) were first

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<sup>1</sup> Pseudo-velocity components can be used to handle other classical degrees of freedom (Macrossan 1995).

selected from a parent distribution having the required mean and variance of the samples. After doing this, the mean value and variance of the samples were not as required (the central limit theorem says that the mean of the sample will be distributed about the mean of the parent distribution). To correct this the velocities were “displaced and rescaled” to ensure that momentum and energy were conserved. As I understand it, their algorithm applied to the fundamental problem of generating a set of  $N$  samples from a normal distribution, with a specified sample mean of 0 and sample variance of 1, could be described as follows:

1. Select  $N$  values,  $x_j, j = 1 \dots N$ , from a parent normal distribution (with **any** mean and **any** variance), by the usual procedures (e.g.  $x_j = [-\ln(R_j)]^{1/2} \cos(T_j)$ , where  $R_j$  and  $T_j$  are uniformly distributed random fractions).
2. Let

$$u_j = (x_j - \bar{x}) / \sigma,$$

where

$$\bar{x} = \sum x_j / N \quad \text{and} \quad \sigma^2 = \sum (x_j - \bar{x})^2 / N$$

Since the mean

$$\bar{u} = \frac{1}{N} \sum u_j = \sum \frac{(x_j - \bar{x})}{N\sigma} = \frac{(\bar{x} - \bar{x})}{\sigma} = 0$$

and the variance

$$s^2 = \frac{1}{N} \sum u_j^2 = \sum \frac{(x_j - \bar{x})^2}{N\sigma^2} = \frac{\sigma^2}{\sigma^2} = 1,$$

and since the  $u_j$  are linearly related to the  $x_j$  selected from a normal distribution, it appears that the  $u_j$  are a satisfactory set of sample values, with a specified sample mean of 0 and specified sample variance of 1. This algorithm appears to work in practice, and requires about 30% of the computational effort of Pullin's formally derived algorithm, mainly because the latter contains elements which inhibit vectorisation. The reduced effort for the above algorithm translates to an increase in speed for the hybrid code of about 1.5 for the test case considered here.

### 3 BREAKDOWN PARAMETER

Bird's breakdown parameter (Bird 1970, 1994) is usually employed in hybrid methods to detect those regions in the flow where DSMC should be invoked. The breakdown parameter

$$P = \tau / t_{flow} \tag{1}$$

is the ratio of the collision time

$$\tau = \lambda / \bar{c} \tag{2}$$

where  $\bar{c}$  is the mean thermal speed, to the flow time

$$t_{flow} = l / v_{char}, \tag{3}$$

the time it takes a molecule moving at characteristic speed  $v_{char}$  to traverse a local characteristic length  $l$ . Thus the breakdown parameter (1) can be expressed as the product of a non-dimensional speed and a non-dimensional length:

$$P_l = \frac{v_{char}}{\bar{c}} \times \frac{\lambda}{l} \tag{4}$$

The local characteristic flow length is usually derived from the local gradients of a flow property  $q$  as

$$l_q = q \left| \frac{\partial q}{\partial x} \right|^{-1}$$

so that

$$P_q = \frac{v_{char}}{\bar{c}} \times \frac{\lambda}{q} \left| \frac{\partial q}{\partial x} \right|. \tag{5}$$

Since the characteristic flow velocity  $v_{char}$ , which is used to derive the characteristic flow time of eq. (3), is the velocity of a typical molecule relative to the flow structures, there is an important distinction to be made between steady and unsteady flows.

- **Steady flow:** For steady flows, the flow structures are stationary, usually fixed relative to a body immersed in the flow, and the characteristic speed of the molecules relative to the flow structures is the mean molecule speed, or local fluid speed,  $v_{char} = \bar{v}$  so that

$$P_q = \frac{\bar{v}}{\bar{c}} \times \frac{\lambda}{q} \left| \frac{\partial q}{\partial x} \right|.$$

If  $q = \rho$ , this is the steady flow version of Bird's breakdown parameter<sup>2</sup>

$$\frac{\lambda}{\bar{c}} \frac{D}{Dt} \log(\rho / \rho_{ref}).$$

- **Unsteady flow:** For unsteady flow where the flow structures are convected with the local flow speed  $\bar{v}$ , the characteristic speed of the molecules, relative to the flow structures, would be closer to the average *thermal speed*  $\bar{c}$ . Putting  $v_{char} = \bar{c}$  in eq. (4), we have

$$P_l = \lambda / l_q$$

which is a local Knudsen number based on the gradient length  $l_q$ .

#### 4 GRADIENT FLOW LENGTHS

It is usual to take  $q = \rho$  but there is a case for making the flow length depend on gradients of temperature as well as density. Two possibilities are to use the gradient of the local mean free path or local mean collision time to derive the local length scale

$$l_\lambda = \lambda \left| \frac{\partial \lambda}{\partial x} \right|^{-1} \quad \text{or} \quad l_\tau = \tau \left| \frac{\partial \tau}{\partial x} \right|^{-1}. \quad (6)$$

Since  $\lambda \propto \mu / (\rho \bar{c})$ , and assuming  $\mu \propto T^\omega$ , we have  $\lambda = a \rho^{-1} T^{\omega-1/2}$  and,  $\tau = b \rho^{-1} T^{\omega-1}$  where  $a$  and  $b$  are constants. The two possibilities for breakdown parameter for unsteady flow, are

$$P_\lambda = \frac{\lambda}{\lambda \left| \frac{\partial \lambda}{\partial x} \right|^{-1}} = \lambda \left| \frac{1}{\rho} \frac{\partial \rho}{\partial x} - (\omega - 1/2) \frac{1}{T} \frac{\partial T}{\partial x} \right| \quad (7)$$

and

$$P_\tau = \frac{\lambda}{\tau \left| \frac{\partial \tau}{\partial x} \right|^{-1}} = \lambda \left| \frac{1}{\rho} \frac{\partial \rho}{\partial x} - (\omega - 1) \frac{1}{T} \frac{\partial T}{\partial x} \right| \quad (8)$$

Note that for hard sphere molecules ( $\omega = 1/2$ ) and for Maxwell molecules ( $\omega = 1$ ),  $P_\lambda$  and  $P_\tau$ , respectively, reduce to the density gradient-length local Knudsen number,

$$Kn_{GL} = \frac{\lambda}{\rho} \left| \frac{\partial \rho}{\partial x} \right|$$

which is the breakdown parameter used successfully by Roveda *et al* (1998) for unsteady flow. In regions of constant pressure, such as in the vicinity of a contact discontinuity, we have  $p = \rho RT = \text{constant}$ , and (7) reduces to

$$P_\lambda = (\omega + 1/2) Kn_{GL} \quad (9)$$

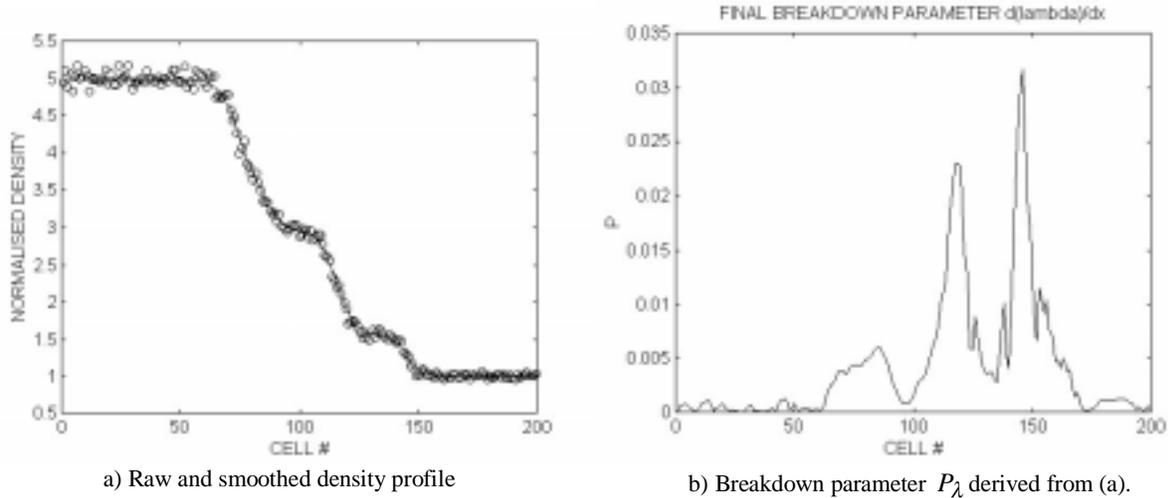
<sup>2</sup> If we assume the local flow time  $l_q / \bar{v}$  is proportional to  $D / u_\infty$ , where  $D$  is a body dimension and  $u_\infty$  is the freestream flow speed, we

can derive a global breakdown parameter based on the freestream conditions as  $P_\infty \approx S_\infty Kn_\infty \approx M_\infty^2 / Re_\infty$ . The parameter  $M_\infty^2 / Re_\infty$  has often been used to establish the onset of rarefied flow (Tsien 48, Schaaf and Chambre 1949, Clayden 1958, Hurlbut 1958).

while (8) reduces to

$$P_\tau = \omega Kn_{GL} \quad (10)$$

Since  $P_\lambda$ ,  $P_\tau$  and  $Kn_{GL}$  are so closely related, there is little reason to prefer one over the others. For this work I have used only hard sphere molecules and  $P_\lambda$ .



**Figure 1.** Smoothed flow properties at time  $tU_s / L_1 = 0.5$ , one run, 80000 particles,  $Kn = 0.01$ .

## 5 TEST CASE - 1D SHOCK TUBE

The unsteady one-dimensional flow in a shock tube was simulated as a test case. In the initial state, a low pressure region (condition 1) extends from  $0 < x < L_1$  and a high pressure region extends from  $-L_2 < x < 0$ . The pressure ratio  $p_2/p_1$  was 5 and the temperature ratio  $T_2/T_1$  was 1. For simplicity the hard sphere collision model was used. The initial Knudsen numbers were  $\lambda_1 / L_1 = 0.01$  and  $\lambda_2 / L_1 = 0.002$ . The cell size was  $\Delta x / L_1 = 0.05$ . Ensemble averages of 20 runs were taken to obtain the final flow state. Each run used 80000 particles.

The time step was  $\Delta t = \tau_1 / 2$ , which was everywhere greater than the local mean free time, except in the undisturbed (uniform) high-pressure gas. The particles in some high density cells will move over distances greater than the local mean free path. However, this should not matter; the flow gradients are negligible and these molecules will have come from a region of last collision where the average flow properties are the same as the region in which they suffer their next collision. This is just another way of saying that the exact values of dissipative coefficients are not important where the flow gradients are negligible.

Figure 1(a) shows a typical raw density profile and the smoothed density profile  $\rho^{**}$  derived from it, as explained below (section 5.1). The boundary between the initial high and low density gas was between cells 100 and 101. The expected features of the unsteady shock tube flow can be seen. Working from the left, there is a region of undisturbed high density gas (cells 1 - 60). From cell 60 to cell 90 (approximately) the density decreases through the unsteady expansion followed by an approximately constant density region (cells 90 - 110). After this there is a “contact region” (cells 110 - 130) where the initial high pressure and low pressure gases mix. The shock in the low density gas is smeared out over cells 140 - 155. The theoretical shock location is at cell 150.

Figure 1(b) shows the breakdown parameter  $P_\lambda(x)$  derived from the smoothed density profile (see section 5.1). The breakdown parameter is negligible in the high density undisturbed gas and larger in the unsteady expansion. It decreases after the expansion before rising dramatically in the “contact region”. It increases dramatically in the interior of the smeared shock.

## 5.1 Smoothed profiles

EPSM is invoked in those cells where  $P_\lambda > P_{crit}$ . Because of the statistical noise in DSMC calculations, the local values of mean free path must be estimated in each cell from smoothed profiles of the macroscopic flow properties. The smoothing process, a simple moving average of the instantaneous flow profiles over a smoothing length  $l_s$ , tends to lessen the flow gradients and hence overestimate the length scale  $l_\lambda$  and under-estimate the breakdown parameter. It is therefore desirable to make the smoothing length as large as possible to eliminate the noise in the profile, but less than the “true” local flow length so that flow gradients are not destroyed by the smoothing.

I have adopted a multi-pass smoothing procedure, which is best explained by writing the algorithm for the general case in which  $\lambda$  is a function of both density and temperature. The final smoothing length is no greater than  $20\lambda^*$  or  $l^*/5$ , where  $\lambda^*$  and  $l^*$  are estimates of the local mean free path and flow length. As a final precaution against noise, I have not used the EPSM in any small regions of “isolated” cells with a length less than  $10\lambda^*$ .

### Smoothing Algorithm

Let  $smth(q(x), l(x))$  be a smoothing function, which returns a “smoothed” profile of the flow property  $q$ , using a smoothing length  $l_s(x)$ . Then:

1. Derive first estimates of the smoothed flow properties

$$\rho^* = smth(\rho, l_s) \text{ and } T^* = smth(T, l_s)$$

with a fixed smoothing length of  $l_s = 6\lambda_1$ .

2. **Derive**  $\lambda^*(x) = f(\rho^*, T^*)$  and the local flow length scale  $l^*(x) = \lambda^* / \left| \partial \lambda^* / \partial x \right|$ .

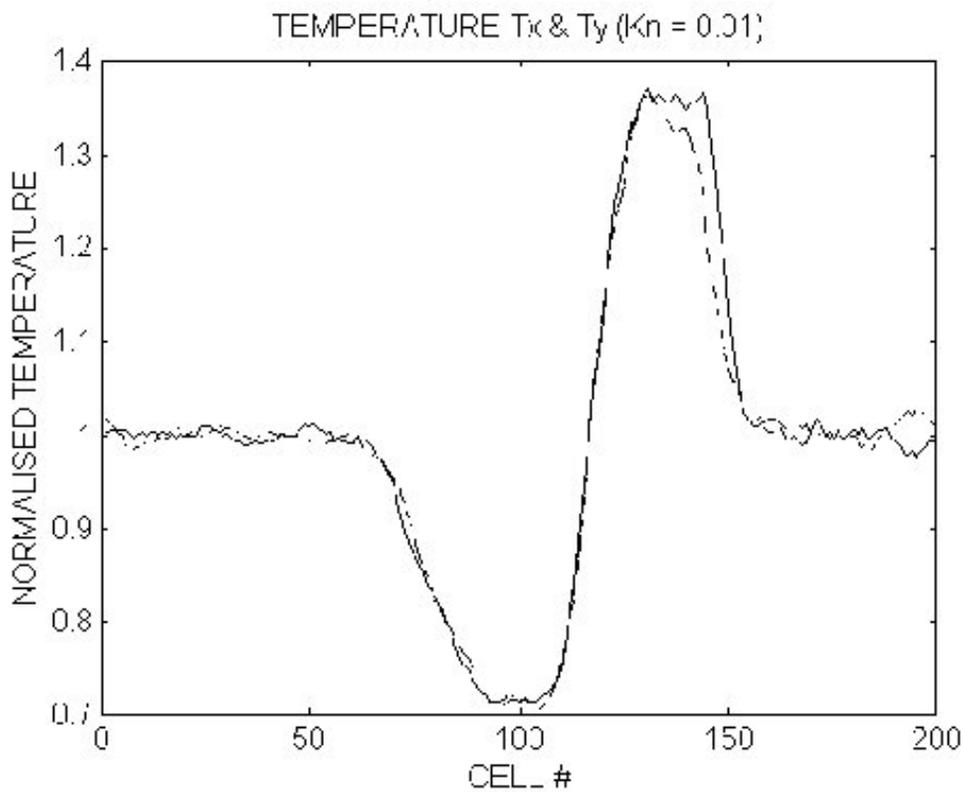
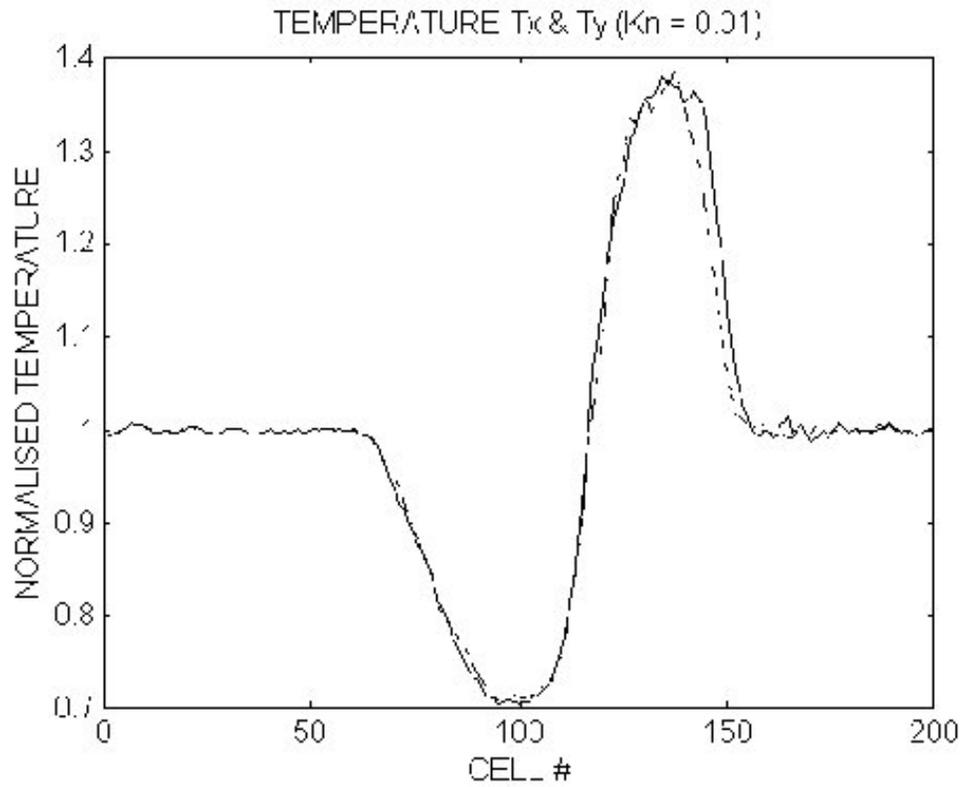
3. Derive second estimates of the smoothed flow properties  $\rho^{**} = smth(\rho, l_s^{**})$  and  $T^{**} = smth(T, l_s^{**})$  with the variable smoothing length  $l_s^{**} = \min(l^* / 5, 20\lambda^*)$ .

4. **Derive**  $\lambda^{**}(x) = f(\rho^{**}, T^{**})$  and the local breakdown parameter  $P_\lambda = \left| \partial \lambda^{**} / \partial x \right|$ .

Typical density profiles and the breakdown parameter derived from the smoothed profiles, were shown in figure 1. There is an element of judgement required to set the value of  $P_{crit}$ . Roveda *et al* (1998) used a critical value of  $Kn_{GL}$  of 0.001. Because the breakdown parameter is derived from smoothed profiles of flow properties, the gradients (and hence the breakdown parameter) will tend to be underestimated. A small value of  $P_{crit}$  is required in order to be conservative (that is, in order to ensure DSMC is used wherever it is required). It can be seen from figure 1(b) that a value of  $P_{crit}$  of 0.001 would ensure that the continuum solver EPSM was used only in the undisturbed gas on both the high and low density sides. I chose a slightly larger value of  $P_{crit} = 0.003$  so that EPSM was used also in the small region between the unsteady expansion and the contact region, where the density gradient is mild. Also, EPSM was occasionally invoked (in some of the ensemble of runs) in the approximately constant density region between the shock and the contact region.

To save computational effort the breakdown parameter is not calculated at every time step. We would not expect the flow properties to change appreciably in one time step if the time step  $\Delta t$  is small with respect to the flow transit time  $t_{cell} = \Delta x / \bar{v}$  or where flow gradients (and hence breakdown parameters) are small. Hence, each time the breakdown parameters are calculated the minimum cell transit time  $t_{min}$  is determined over the DSMC regions only. The computational grid is not divided into DSMC and EPSM regions again until a further simulated time of  $0.5t_{min}$  has elapsed.

Figure 2(a) shows the normalized temperature profiles,  $T_x/T_1$  and  $T_y/T_1$  obtained with the hybrid method, for an elapsed flow time of  $L_l/(2U_s)$ , where  $U_s$  is the theoretical shock speed. Figure 2(b) shows the corresponding temperature profiles for DSMC. In general the results are the same; the non-equilibrium state (as shown by the differences between  $T_x$  and  $T_y$ ) in the shock and expansion region is captured by the DSMC part of the hybrid method. It is interesting to note that DSMC seems to show a slight degree of non-equilibrium in the “undisturbed”



**Figure 2** Temperature profiles  $T_x/T_1$ ,  $T_y/T_1$ ,  $tU_x/L_1=0.5$ ,  $Kn_1=0.01$ . Ensemble averaged,  $20 \times 8000$  particles

gas at both ends of the shock tube, whereas for any cell where EPSM was always used there can be no difference between the temperature components. The DSMC results here would normally be interpreted as statistical “error”. This makes it difficult to interpret the small differences between pure DSMC and hybrid EPSM/DSMC in the region between the shock and the contact region – it could also be statistical error in DSMC that produces the slightly large departure from equilibrium here. The flow gradients are small here and occasionally EPSM has been invoked in these cells (see the small values of  $P_\lambda$  in this region for one run of the ensemble shown in figure 1(b)).

## CONCLUSIONS

A particle based hybrid method has been presented and shown to offer computational advantages over pure DSMC for a test flow with a Knudsen number of 0.01. Pullin’s Equilibrium Particle Simulation Method (EPSM) has been shown to be sufficiently accurate for those regions of the flow where equilibrium conditions can be expected. The interface between the DSMC and EPSM regions of the flow presents none of the difficulties usually associated with hybrid continuum/DSMC solvers. The hybrid code apparently produces less scatter in the temperature in regions of undisturbed flow.

A distinction has been drawn between the appropriate form of the breakdown parameter for an unsteady flow (as here) and a steady flow. In the former case, the flow structures (or flow gradients) can be convected with the flow so the characteristic particle speed relative to the flow structures is the local thermal speed. In that case the breakdown parameter reduces to a local Knudsen number based on gradients of flow properties. It is convenient to derive the local flow lengths from the gradients of mean free path, which depends in general on temperature and density gradients. For unsteady flow the breakdown parameter then reduces to  $|\partial\lambda/\partial x|$ .

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