JOURNAL OF COMPUTATIONAL PHYSICS 8, 309–310 (1971)

Letter to the Editor

Comments on "Simulation of Relaxation Processes by Monte Carlo"

Matthes [1] has recently outlined a Monte Carlo procedure for the computation of representative molecular collisions in a simulated gas. Step (2) of his procedure requires the summation of the product of collision cross section and relative velocity over all pairs of particles in the gas. This step is repeated after the calculation of each collision and is almost certainly the dominant factor in determining the computing load. The purpose of this note is to point out that the step is unnecessary and has been avoided in a Monte Carlo procedure [2] that has previously been applied to this problem.

The summation also appears in Matthes' Eq. (5) for the distribution W_{ik} which is used in his Step (3) for the selection of collision pairs. However, it is a constant in the instantaneous value of this distribution and the only requirement for the selection of collision partners is that the probability of selection of a particular pair should be proportional to the product of their relative velocity and cross section. The key point is that the time may be advanced at each collision by an amount that also depends only on the relative velocity and cross section of the particular pair of molecules in the collision, as outlined in [2]. The summation in Matthes' procedure effectively calculates the mean collision time, but this has been shown [2] to be automatically established when the simpler procedure is applied over a large number of collisions.

The simple Monte Carlo procedure was first applied to the translational relaxation problem in 1963 [3]. In that case, the establishment of a time parameter directly related to real time was avoided by presenting the results as a function of the mean collision rate. However, such a time parameter has been used in all subsequent applications to multidimensional problems (for example, [4, 5]) and in recent [6] calculations of relaxation in gases with internal degrees of freedom and chemical reactions. The latter calculations permit a direct comparison of computing requirements, in that for the simplest relaxation problem corresponding to Matthes' "Application A," an IBM 360/75 computed at a rate of 50 000 collisions per minute. Moreover, a sample of 4000 particles used only a fraction of the available core, and the restriction to 100 particles in [1] indicates that it was found necessary to store some of the products for summation rather than recalculate them at each step. The avoidance of the repeated summation appears to increase both the computing speed and allowable sample by a factor of 40.

REFERENCES

1. W. MATTHES, *J. Comput. Phys.* **6** (1970), 157.
2. G. A. BIRD, *Phys. Fluids*, **13** (1970), 2676.
3. G. A. BIRD, *Phys. Fluids*, **6** (1963), 1518.
4. F. W. VOGENITZ, G. A. BIRD, J. E. BROADWELL AND H. RUNGALDIER, *AIAA J.* **6** (1968), 2388
5. G. A. BIRD, *J. Fluid Mech.* **36** (1969), 571.
6. G. A. BIRD, "Numerical Simulation and the Boltzmann Equation," Proc. 7th International Symposium on Rarefied Gas Dynamics, to be published.

RECEIVED: January 4, 1971

G. A. BIRD,

Department of Aeronautical Engineering,
University of Sydney, Sydney, Australia 2006