The initial condition, NO, was defined as follows (Fortran Notation):

```
NO=6.023E23*(1+0.1*COS(PI*X))
 *EXP(-(VX/1.E3)**2)/(SORT(PI)*1.E3)
 *EXP(-(VY/1.E3)**2)/(SORT(PI)*1.E3)      (1)
      where PI=3.14159
```

Note that the initial disturbance in the gas is spacial. It does not involve the velocity functions.

THE INTERACTION

TRANSFORMATION TO CENTER-OF-MASS COORDINATES

The first step in analyzing the interaction between two colliding particles is to transform VX and VY into center-of-mass (C.M.) coordinates. For each of the velocity variables, the velocity of the center-of-mass and the velocity about the center-of-mass is given by (2) and (3). Its inverse is defined by (4) and (5).

$$VC=(V1+V2)/2 \qquad (2)$$

$$VO=(V1-V2)/2 \qquad (3)$$

$$V1=VC+VO \qquad (4)$$

$$V2=VC-VO \qquad (5)$$

According to (2) and (3), if $-1000 <= V1 <= 1000$ and $-1000 <= V2 <= 1000$, then $-1000 <= VC <= 1000$ and $-1000 <= VO <= 1000$. According to (4) and (5), if $-1000 <= VC <= 1000$ and $-1000 <= VO <= 1000$ then $-2000 <= V1 <= 2000$ and $-2000 <= V2 <= 2000$. When using (4) and (5) to transform a probability density function into C.M. coordinates, extrapolation must be used to extend the range of V1 and V2.

Two operators were defined to perform the transformation of (4) and (5) upon the log of the probability function. For those values of VO and VC where $-1000 <= V1$, $V2 <= 1000$, the associated operator performed interpolation. For other points, the operator performed extrapolation. An examination of (4) and (5) will show that the points of interpolation result in values of V1 and V2 which are equal to the knots of VX and VY. Hence there are no errors of interpolation.

Before transformation into C.M. coordinates, N(X,VX,VY,T) was separated into a NX(X,T), NVX(X,VX,T), AND NVY(X,VY,T) such that:

$$N=NX*NVX*NVY \qquad (6)$$

It was assumed that N was sufficiently "Gaussian" (no cross terms between VX and VY) to permit this decomposition. This decomposition greatly reduced the quantity of data being processed.

Applying the transformation (4) and (5) to NVX(X,VX,T) and NVY(X,VY,T) resulted in NVXCO(X,VXC,VXO,T) and NVYCO(X,VYC,VYO,T). Again, NVXCO(X,VXC,VXO,T) and NVYCO(X,VYC,VYO,T) were separated into NVXC(X,VXC,T), NVXO(X,VXO,T) and NVYC(X,VYC,T), NVYO(X,VYO,T) respectively.

TRANSFORMATION ACROSS THE INTERACTION

The selected interaction between particles was the collision of two hard spheres. Rotation of the interacting molecules was ignored. This interaction creates a rotation of the velocity vectors of the two colliding particles relative to the center-of-mass. This rotation is expressed as follows:

$$VOX1=-VOX2*COS(THETA)+VOY2*SIN(THETA) \qquad (7)$$

$$VOY1=-VOX2*SIN(THETA)-VOY2*COS(THETA) \qquad (8)$$

where VOX1 and VOY1 represent the particle before the interaction, VOX2 and VOY2 represent the particle after the interaction, and THETA is twice the angle of impact. Setting $-1000 <= VX02, VY02 <= 1000$ in (7) and (8), VOY1 and VOX1 will exceed the limits of VOX, VOY. Again extrapolation was required for some of the combinations of VOX2, VOY2 and THETA.

To achieve a better approximation, the transformation defined by (7) and (8) was applied to the log of the functions NVXO(X,VXO1,T) and NVYO(X,VYO1,T). The resultant functions were combined with the probability of a specific interaction to form a composite function of X, VXO2, VYO2, T, and THETA. The resultant function was integrated with respect to THETA and then separated into two functions NVXO1(X,VXO2,T) and NVYO1(X,VYO2,T).

A set of composite operators were prepared for this transformation. First, operators were defined to expand the variable range of VOX, VOY by substituting a 9 point dummy variable, $-2000 <= d <= 2000$. Both extrapolation and interpolation was employed with the interpolated points being equal to the knots of the replaced variable. Second, operators to replace the dummy variable with the results of (7) and (8) were defined. These operators were then applied to the first set of operators to form the composite operators. In this manner, interpolation errors near the end-points were minimized.

TRANSFORMATION TO CARTESIAN COORDINATES

The third step is to transform NVXO2, NVYO2, NVXC, NVYC back to cartesian coordinates. Equations (2), (3) were used; and hence, extrapolation does not appear to be needed. However, the end-point errors of the spline approximation were again encountered. Hence, to achieve the desired accuracy, (integral of resultant probability function equal to one +/- 0.1%), it was necessary to use a dummy variable, $-2000 <= d <= 2000$ as before and then apply interpolation. Composite operators were again defined to perform this functional substitution upon the log of the probability functions.

Equations (2), (3) will transform VXC, VXO2 and VYC, VYO2 into the velocities of interacting particles, VX1, VY1, VX2, and VY2, and the probability functions NVYO1, NVXO1, NVYC, NVXC into NVX3(X, VX1, VX2,T) and NVY3 (X,VY1,VY2,T). The two particles are identical. NVX3 is separated into functions of NVX31(X,VX1,T) and NVX32 (X,VX2,T) which are summed to form NVX1(X,VX,T). NVY1(X,VY,T) is similarly computed from NVY3.

COMPUTATION OF A COLLISION RATE FUNCTION

Recall that N was separated into NX, NVX, NVY. The time dependency of NX will be developed later. RVX and RVY, the rate of change in NVX and NVY, will be computed as follows:

$$RVX=(NVX1-NVX)*F \qquad (9)$$

$$RVY=(NVY1-NVY)*F \qquad (10)$$

where F, the collision frequency, is the product of the mean velocity, cross-section, and NX.

SOLUTION OF DIFFERENTIAL EQUATION

TRANSFORMATION TO MOVING COORDINATES

The Lliouville equation for this experiment is as follows:

$$[dN/dX]*VX+[dN/dVX]*AX+[dN/dVY]*AY+[dN/dT]+RC=0 \qquad (11)$$

where the bracketed items are partial derivatives, AX, AY are accelerations equal to zero, and RC is the rate of change of N due to interactions. Substituting the zeros yields: