A VELOCITY DISTRIBUTION MODEL FOR STEADY STATE HEAT TRANSFER

Final Report
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ABSTRACT

Consider a box that is filled with an ideal gas and that is aligned along Cartesian coordinates (x, y, z) having until length in the "y" direction and unspecified length in the "x" and "z" directions. Heat is applied uniformly over the "hot" end of the box ($y = 1$) and is removed uniformly over the "cold" end ($y = 0$) at a constant rate such that the ends of the box are maintained at temperatures T_0 at $y = 0$ and T_1 at $y = 1$. Let U, V, and W denote the respective velocity components of a molecule inside the box selected at some random time and at some location (x, y, z). If $T_0 = T_1$, then U, V, and W are mutually independent and Gaussian, each with mean zero and variance RT_0, where R is the gas constant. When $T_0 \neq T_1$ the velocity components are *not* independent and are *not* Gaussian. Our objective is to characterize the joint distribution of the velocity components U, V, and W as a function of y, and, in particular, to characterize the distribution of V given y. It is hoped that this research will lead to an increased physical understanding of the nature of turbulence.

THE SIMULATION

Consider a box that is filled with an ideal gas and that is aligned along Cartesian coordinates (x, y, z) having until length in the "y" direction and unspecified length in the "x" and "z" directions. Heat is applied uniformly over the "hot" end of the box (y = 1) and is removed uniformly over the "cold" end (y = 0) at a constant rate such that the ends of the box are maintained at temperatures T_0 at y = 0 and T_1 at y = 1. Let U, V, and W denote the respective velocity components of a molecule inside the box selected at some random time and at some location (x, y, z). (See Figure 1.) Our concern in this project is to characterize these velocity components. In this regard, we will first consider the problem of simulating the molecular motion inside the box so as to obtain simulated velocities. This simulation will be based on the direct simulation Monte Carlo code presented in [Bird, 1994].

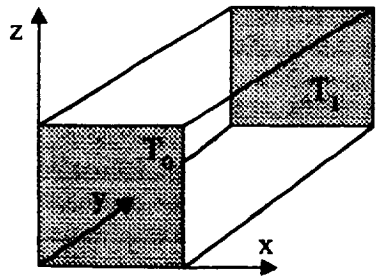


Figure 1

For the simulation, we will consider (as indicated by Figure 2) a thin slice of the box that effectively ignores the z spatial component. The z component is not entirely neglected however since the molecule velocities are considered three dimensional even though the molecule positions are taken to be only two dimensional. This two dimensional slice is divided into cells and subcells as indicated by Figure 3. As Bird describes the problem in [Bird, 1994, p. 215], subcells were introduced because it "was feared that coincidental collisions between molecules at opposite sides of the cells, coupled with the immediate migration of these molecules to the next cell, might cause false disturbances to propagate with speed equal to the ratio of the cell size to the time step."

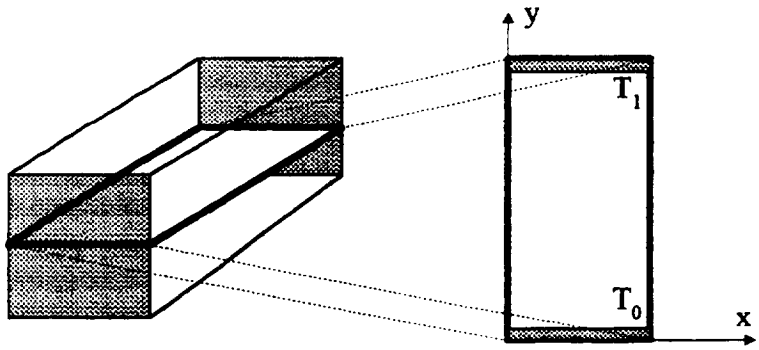


Figure 2

In order to explain the operation of the simulation program, we will consider the input file `dsmc2.dat` that contains the data used to produce a particular simulation run. Any line in the data file beginning with '#' is treated as a comment and is ignored by the program. The line numbers mentioned below refer to the copy of this file that is reproduced at the end of this report.

The first item in the file (lines 6-9) determines whether or not an output file `dsmc2.out` is produced. This file corresponds to the only output provided by the original program `dsmc2.for` from [Bird, 1994].

When the program begins, it first asks whether a new calculation is desired or an old calculation should be restarted. This latter option is only possible when line 19 of the data file has been set to 0 in an earlier run in order to produce a restart file. The restart file `dsmc2.res` contains a snapshot of the current state of the simulation and can be used to restart the program at that point should any sort of interruption occur. (Note that the size of this restart file can be as large as 20 Meg.) For long simulations, it is suggested that the values in lines 19-20 be chosen so that a restart file is produced approximately once each hour. Producing the file more frequently may greatly reduce the speed of the simulation.

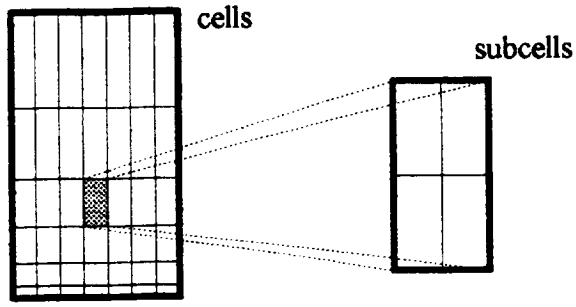


Figure 3

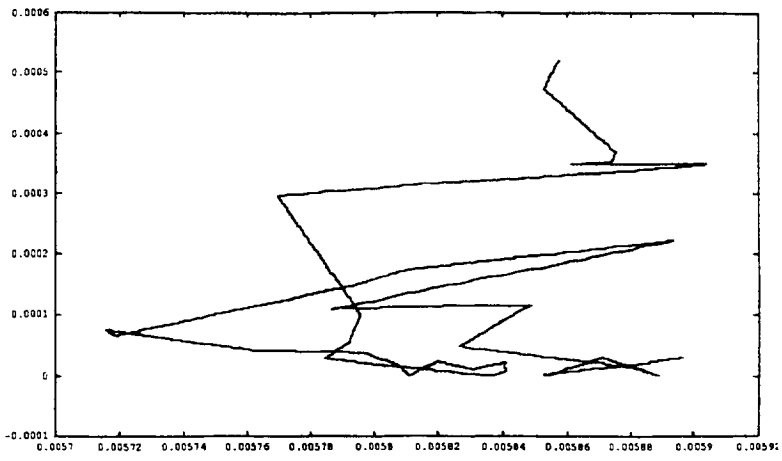
A second output option is the production of a log file `dsmc2.log` that contains velocity and temperature information for cells along a particular y location. This file is produced when line 26 of the data file is set to zero. The value for y is specified by line 150 of the input file. In addition, this log file contains information regarding the number of molecules per cell that may be useful is choosing a proper value of *CWRY*, which is considered below. A sample of this output file is given near the end of this report. Note that the averages given by this option are not cumulative but are instead based only on the number of molecules occupying cells along the given y location at the time the file is updated.

The next output option determines whether or not a chart of velocity moments is produced during the simulation. When this option is selected by setting line 31 of the data file to zero, a chart as given later in this report is periodically written to the screen and to the file `dsmc2.cht`. The statistics in this chart are cumulative over the run of the simulation. The third column indicates the total number of molecules that have been used to obtain the sample moments found in the final three columns. The row numbers that are used to produce the chart are determined by lines 163-182 of the data file. Note that it is possible to produce this data for every row in the box simply by setting line 167 in the data file equal to the total number of rows in the box.

A third output option makes it possible to track the position of a molecule initially located along some specified row. A file called `dsmc2.mol` containing the (x, y) coordinates of a molecule in the specified row is produced when line 36 of the data file is set to zero. The initial molecule row number is specified by line 154 of the data file. Since the molecules generally move only slightly between successive time steps, the step size provided

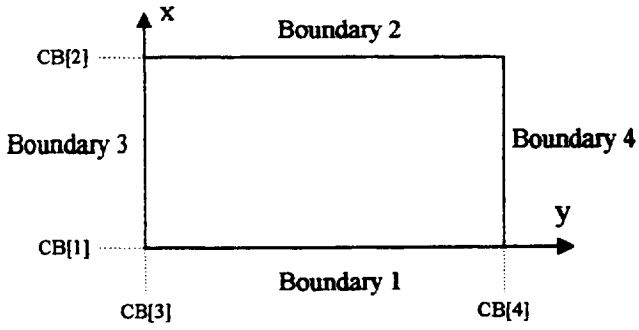
by line 161 makes it possible to more easily obtain a picture of the molecule's motion over a longer period of time.. A graph that shows how the data file `dsmc2.mol` can be used to study the molecular motion produced by the simulation is given below.

The cell widths in the y direction are not uniform, but instead are chosen to be smaller at the cold end of the box than at the hot end of the box. The ratio CWRY of the cell width at the hot end of the box to the cell width at the cold end is given in line 40 of the data file. If $S = CWRY^{1/199}$, then the width of the cell in Row i is given by $WS^{i-1}(1-S)/(1-S^{200})$ where W is the total width of the box in the y direction. Note that here we have assumed that the total number of rows in the y direction is 200. This value can be changed if the code is recompiled. Generally, the ratio *CWRY* should be the square root of the ratio of the temperatures at the two ends of the boxes. A graph showing the number of molecules in each row for a particular simulation is given near the end of this report.



The initial temperature of the gas is determined by *FTMP*, which we have chosen to be the geometric mean of the two surface temperatures. This value is given in line 44 of the data file. The initial number density *FND* is in molecules per square meter. This value is specified in line 48 of the data file.

In the DSMC method, a single simulated molecule represents *FNUM* actual molecules. This value is given in line 52 of the data file and must be chosen so that the total number of simulated molecules is not greater than the maximum allowed number of molecules, which in this case is 40000. (This value can be changed if the code is recompiled.) The actual number of simulated molecules used by the program is given by (*FND/FNUM*) multiplied by the area of the box.



.Figure 4

The value *DTM* in line 56 of the data file is the time step of the simulation, and it should be chosen so that the molecular motion and the collisions are uncoupled. In particular, it should be much less than the local mean collision time. The DSMC

method becomes increasingly more accurate as the cell size and the time step tend to zero. (See [Bird, 1994, p. 215].)

The values $CB[i]$ for i = 1, 2, 3, and 4, are specified in lines 69-81 of the data file and determine the dimensions of the box as indicated by Figure 4. Two planar surfaces (Surface 1 and Surface 2) at possibly different temperatures may be placed anywhere within the box. The reflection at these surfaces is diffuse, which means that the return velocity of a colliding molecule is determined by the temperature of the wall instead of by the incident velocity. At the walls (or boundaries) of the box, the reflection is specular, which means that the appropriate velocity component before the collision is simply reversed to obtain the velocity component after the collision.

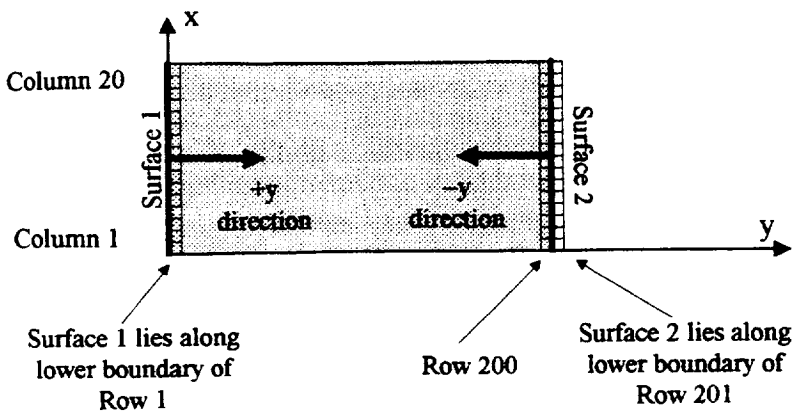


Figure 5

Surface 1 is specified by the parameters in lines 92-110 of the data file. The value *ISURF*[1] specifies the direction of a line normal to the surface and pointing toward the gas. For specular reflection, it is this velocity component that is reversed upon reflection. (The velocity components parallel to the surface are not changed.) For example, in Figure 5, such a normal is in the positive y direction, which corresponds to a value of 1 for *ISURF*[1]. The negative y direction corresponds to a value of 2, the positive x direction corresponds to a value of 3, and the negative x direction corresponds to a value of 4. The values of *LIM*[1][i] specify the location of Surface 1 as indicated by Figure 5 and the descriptions in lines 96-106 of the data file. The value *TSURF*[1] is the temperature of Surface 1. Surface 2 is similarly specified by the parameters in lines 112-130.

The values in lines 132-146 determine the rate of output and the duration of the simulation. Their use is illustrated by the flow chart near the end of this report. Note that the sampling does not begin until *NPS* output cycles have occurred. The moment chart is not produced until this same point is reached.

FUTURE DIRECTIONS

The ultimate goal of this work is to characterize the conditional distribution of the y component of the velocity given a particular location y. Since this problem appears to be

analytically intractable, any practical investigation of the distribution will involve data obtained either empirically or via a simulation such as the one that we have considered here.

One immediate item for future consideration involves the effect of the random number generator on the simulation results. We, as did Bird, have used the algorithm by Knuth that is found in [Press *et al.*, 1992, p. 283]. In [Ferrenberg *et al.*, 1992], it was shown that subtle numerical errors can occur in Monte Carlo simulations when many supposedly 'good' random number generators are used. Since our simulation requires a *large* number of random numbers, it would be helpful to repeat and compare these simulations with a variety of different random number algorithms.

A second item for future consideration involves an investigation of the boundary conditions at the two surfaces. The current code assumes that the distribution of the velocity component that is normal to the surface has the form of a zero mean Gaussian distribution taken to the right of the origin and renormalized. This is the distribution that would correspond to molecules crossing the surface from some external stationary equilibrium gas. (See [Bird, 1994, p. 259].) An alternate model that provides a better fit with the simulated data is a distribution obtained by taking the absolute value of the difference of two independent gamma random variables.

REFERENCES

Bird, G. A., *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*, Clarendon Press, Oxford, 1994.

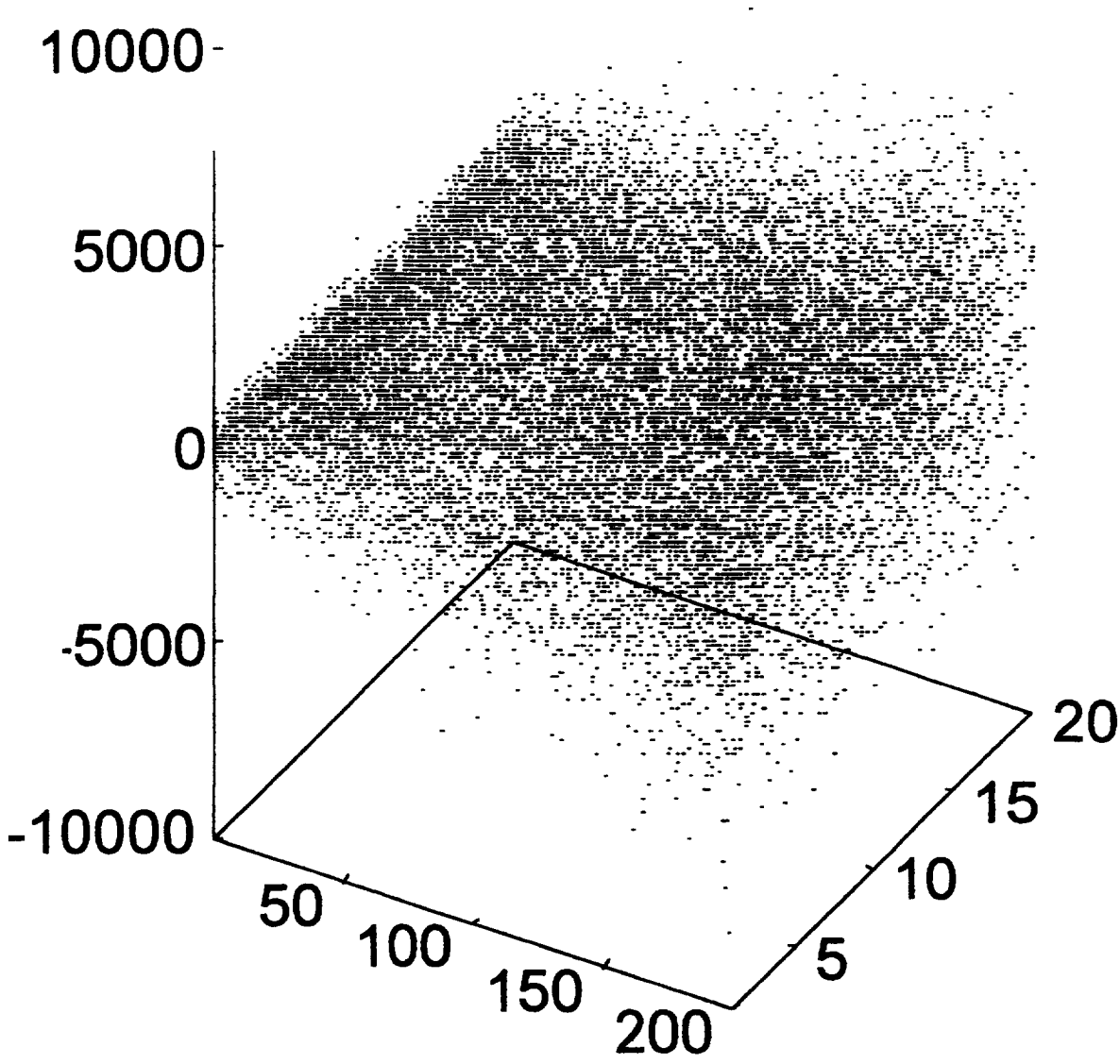
Chapman, S., and T. G. Cowling, *The Mathematical Theory of Non-Uniform Gases*, Third edition, Cambridge University Press, Cambridge, 1970.

Ferrenberg, A. M., D. P. Landau, and Y. Joanna Wong, "Monte Carlo Simulations: Hidden Errors from 'Good' Random Number Generators," *Physical Review Letters*, Vol. 69, No. 23, Dec. 7, 1992, pp. 3382–3384.

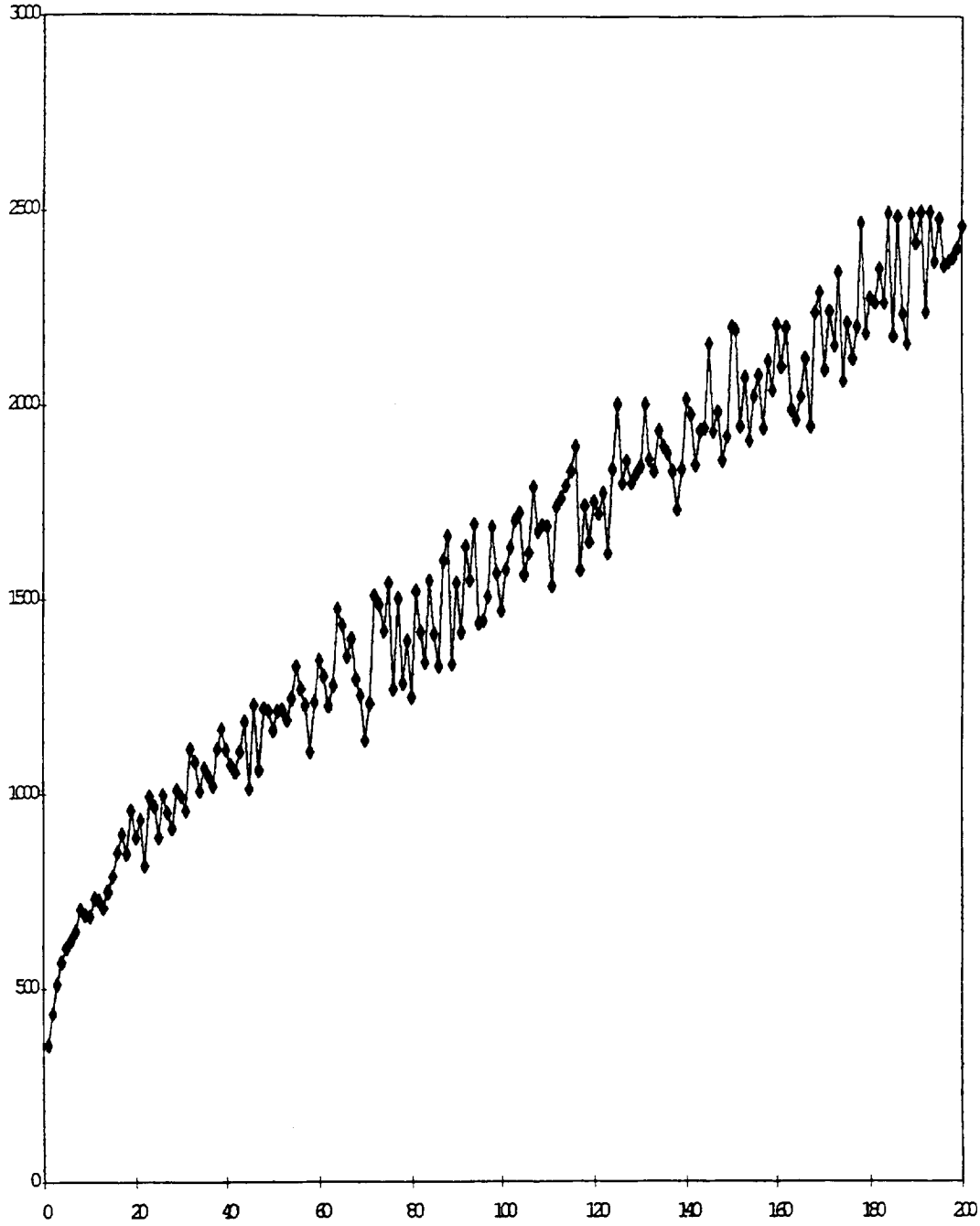
Meyer, R. E., *Introduction to Mathematical Fluid Dynamics*, Dover Publications, New York, 1971.

Press, W., S. A. Teukolsky, W. T. Vetterling, B. P. Flannery, *Numerical Recipes in C: The Art of Scientific Computing*, Second edition, Cambridge University Press, 1992.

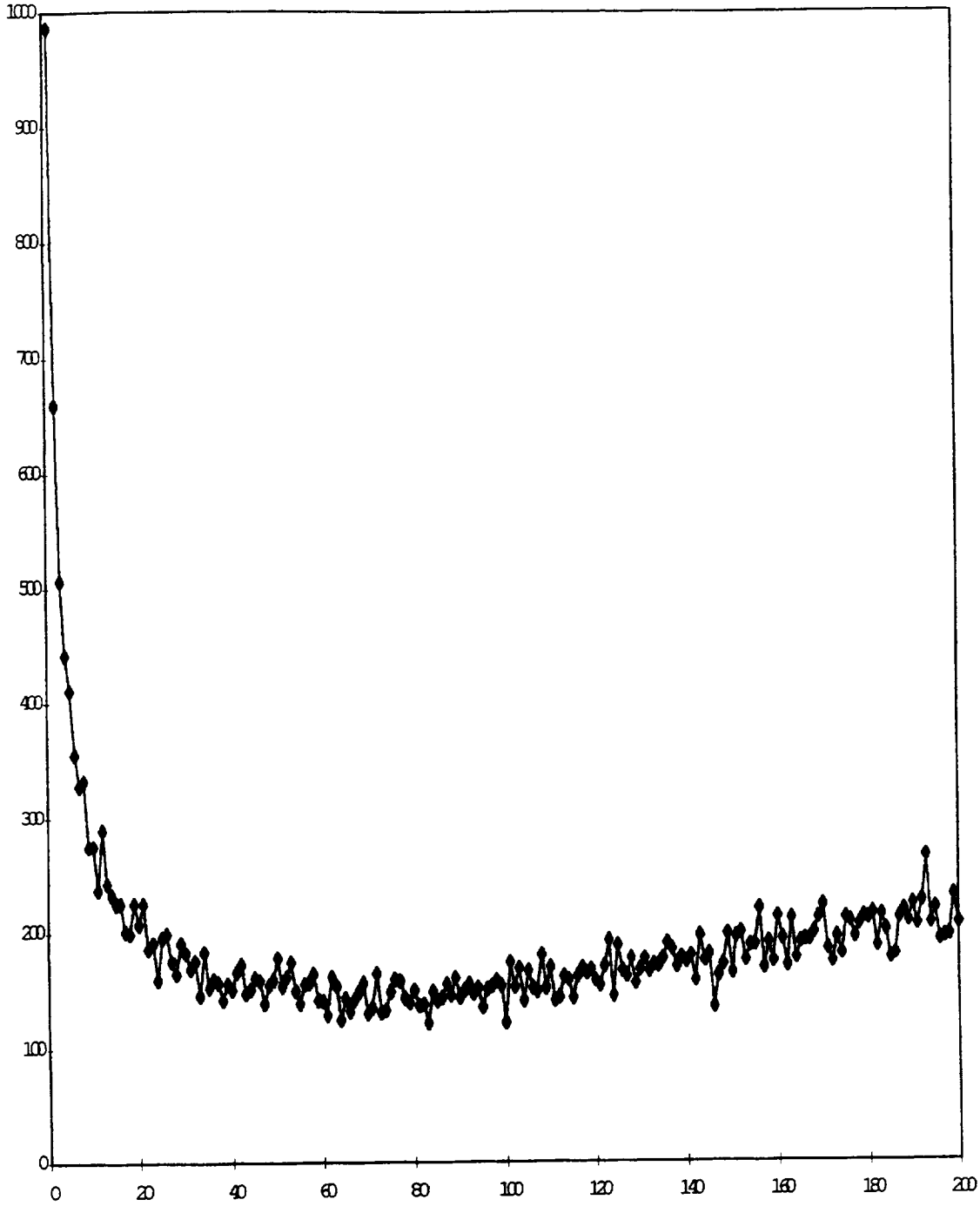
Prigogine, I., "Evolution Criteria, Variational Properties, and Fluctuations," *Nonequilibrium Thermodynamics: Variational Techniques and Stability*, University of Chicago Press, Chicago, 1966, pp. 3-16.



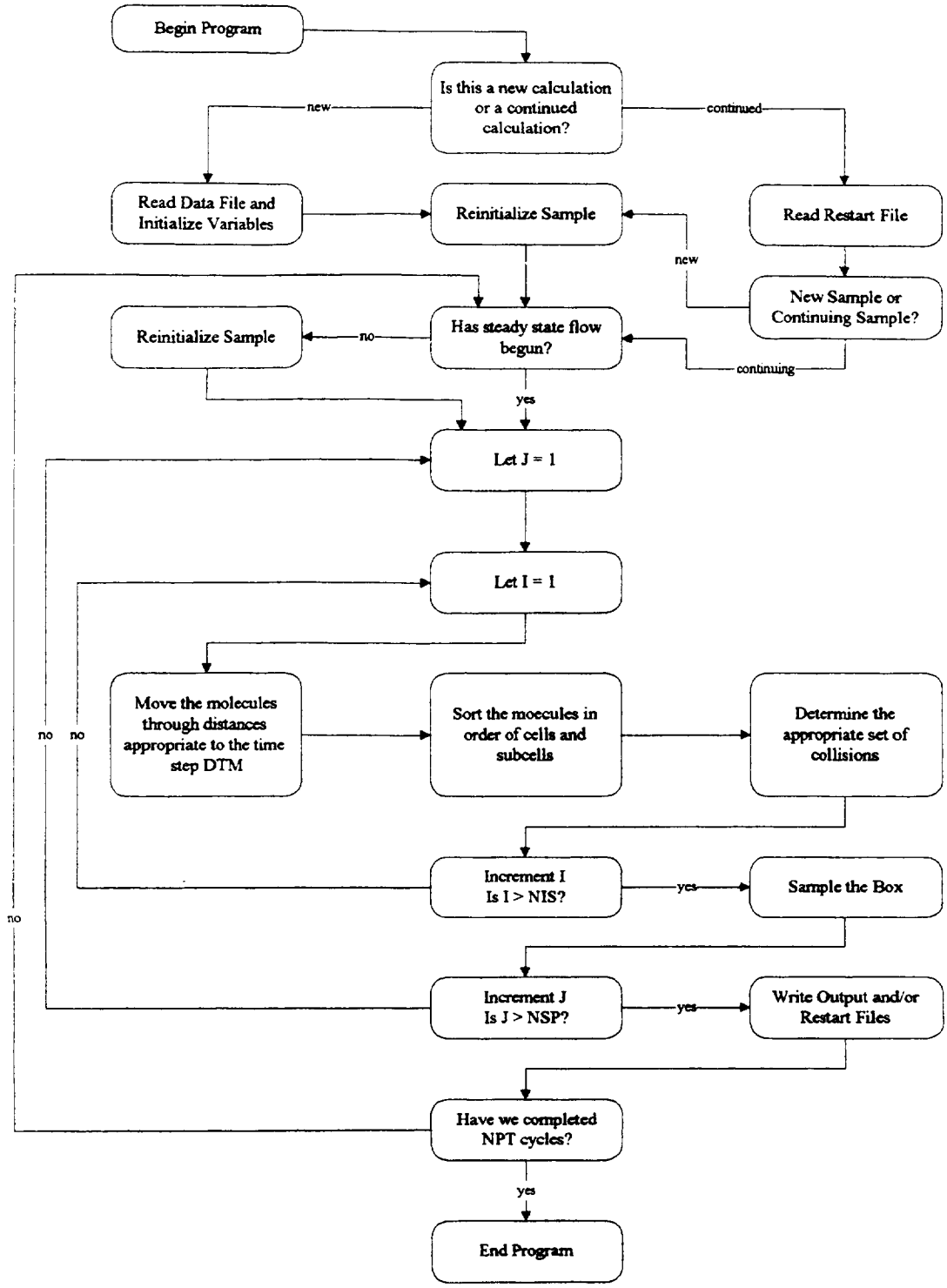
Scatter plot of y velocity component in meters/second for approximately 16000 molecules selected at random from the box after approximately 268 million collisions have occurred. The temperature at row 1 is 300 and at row 200 is 30000.



A plot of the root mean square value of the *y* velocity component for each row in the box. Again, the values were obtained for a box that had experienced approximately 268 million simulated collisions. The temperature at row 1 is 300 and at row 200 is 30000.



A plot of the number of molecules present in each row of a box that has experienced approximately 268 million simulated collisions. The cell width at row 200 is ten times the cell width at row 200.


Begin Program
Is this a new calculation or a continued calculation?
new
continued
Read Data File and Initialize Variables
Reinitialize Sample
Read Restart File
new
New Sample or Continuing Sample?
Reinitialize Sample
no
Has steady state flow begun?
continuing
yes
Let J = 1
Let I = 1
Move the molecules through distances appropriate to the time step DTM
Sort the moecules in order of cells and subcells
Determine the appropriate set of collisions
no
no
Increment I
Is I > NIS?
yes
Sample the Box
no
Increment J
Is J > NSP?
yes
Write Output and/or Restart Files
Have we completed NPT cycles?
yes
End Program

```
**************************************************
Log Update 94
37538 Molecules and 432153 Collisions
Average molecules per cell    = 9.4
Maximum molecules per cell    = 37
Minimum molecules per cell    = 0
Percentage of nonzero cells   = 99%
Data for cells along line y   = 0.005840
Total number of molecules     = 176
Average Temperature of Cells =    2932.75
Average U velocity component = 0.04133742 km/s
Average V velocity component = 0.002432757 km/s
Average W velocity component = -0.002770768 km/s
Average Squared U vel compt  =  0.5711446
Average Squared V vel compt  =   0.719397
Average Squared W vel compt  =  0.6397187
Average U^3 velocity compt   =   0.101235
Average V^3 velocity compt   = 0.01372038
Average W^3 velocity compt   = -0.04497306
Average U^4 velocity compt   =  0.9689213
Average V^4 velocity compt   =    1.44099
Average W^4 velocity compt   =    1.14349
Average X Component of Mol   = -0.0002265342
Average Y Component of Mol   = 0.005869242
```

Sample of `dsmc2.log`

```
Molecules    = 37538
Collisions   = 145790602
Start Time   = 1.16e-06
End Time     = 0.00055648
DTM          = 2e-09
FNUM         = 1.3e+14
CWRY         = 10
FTMP         = 3000
FND          = 0
Surf 1 Temp = 300
Surf 2 Temp = 30000

  Row  Y Midpoint    Mol Count   2nd Moment  3rd Moment  4th Moment
   20  0.00055534     2874478       0.7194     -0.2035      1.7523
   40  0.00127118     2260561       1.1495     -0.3343      4.3424
   50  0.00169623     2158229       1.3561     -0.3945      6.0186
   60  0.00217341     2103919       1.5588     -0.4584      7.9019
   80  0.00331058     2086605       1.9812     -0.5631     12.6606
  100  0.00474384     2146617       2.4251     -0.7288     18.9076
  120  0.00655029     2246682       2.9223     -0.8890     27.4045
  140  0.00882712     2378198       3.4810     -1.0843     38.6212
  160  0.01169679     2527745       4.1265     -1.3110     53.6066
  180  0.01531368     2695610       4.8761     -1.5899     73.5440
```

Sample of `dsmc2.cht`

```
#-----------------------------------------------------------------------
# DATA FILE FOR DSMC2
# Any line beginning with '#' is ignored.
# Data should be placed on a single line following each description.
#-----------------------------------------------------------------------
# 1: Do not produce an output file
# 0: Produce output files
#-----------------------------------------------------------------------
1
#-----------------------------------------------------------------------
# 1: Do not produce a restart file
# 0: Produce a restart file at every Nth output file
# The value of N should follow the flag value below.
# For example, if the next two data lines were
#       0
#       5
# then a restart file would be produced after each group of 5 outputs.
#-----------------------------------------------------------------------
0
100
#-----------------------------------------------------------------------
# 1: Do not produce a log file
# 0: Produce a log file whenever an output file is produced
# See Y Value below
#-----------------------------------------------------------------------
1
#-----------------------------------------------------------------------
# 1: Do not produce a moment chart
# 0: Produce a moment chart whenever an output file is produced
#-----------------------------------------------------------------------
0
#-----------------------------------------------------------------------
# 1: Do not produce a molecule track file
# 0: Track a molecule in row specified below
#-----------------------------------------------------------------------
0
#-----------------------------------------------------------------------
# CWRY: Ratio of cell width at outer to that at inner y boundary
#-----------------------------------------------------------------------
10
#-----------------------------------------------------------------------
# FTMP: The stream temperature
#-----------------------------------------------------------------------
3000
#-----------------------------------------------------------------------
# FND: The initial number density
#-----------------------------------------------------------------------
1.22e22
#-----------------------------------------------------------------------
# FNUM: The number of real mols represented by each simulated mol
#-----------------------------------------------------------------------
0.13e15
#-----------------------------------------------------------------------
# DTM: The time step over which mol motion and collisions are uncoupled
#-----------------------------------------------------------------------
2e-9
#-----------------------------------------------------------------------
#                                  Boundary 2
#              high x ------------------------------
#                     |                              |
#          Boundary   |                              | Boundary
#             3       |                              |     4
```

```
63 | #                        |                                |
64 | #                  low x ------------------------------
65 | #                        low y     Boundary 1      high y
66 | #-------------------------------------------------------------------------
67 | # CB[1]: The x coordinate of boundary 1 (low x)
68 | #-------------------------------------------------------------------------
69 | -0.01
70 | #-------------------------------------------------------------------------
71 | # CB[2]: The x coordinate of boundary 2 (high x)
72 | #-------------------------------------------------------------------------
73 | 0.01
74 | #-------------------------------------------------------------------------
75 | # CB[3]: The y coordinate of boundary 3 (low y)
76 | #-------------------------------------------------------------------------
77 | 0
78 | #-------------------------------------------------------------------------
79 | # CB[4]: The y coordinate of boundary 4 (high y)
80 | #-------------------------------------------------------------------------
81 | 0.02
82 | #-------------------------------------------------------------------------
83 | #
84 | #                  Col 20 ------------------------------
85 | #                         |                            |
86 | #                 Surface |----> pos y       neg y <----| Surface
87 | #                    1    |       dir         dir       |    2
88 | #                         |                             |
89 | #                  Col 1  ------------------------------
90 | #                        Row 1                        Row 200
91 | #-------------------------------------------------------------------------
92 | # ISURF[1]: Direction of surface 1 normal is in the positive y direction
93 | #-------------------------------------------------------------------------
94 | 1
95 | #-------------------------------------------------------------------------
96 | # LIMS[1][1]: Surface 1 lies along lower boundary of this row
97 | #-------------------------------------------------------------------------
98 | 1
99 | #-------------------------------------------------------------------------
100 | # LIMS[1][2]: Surface 1 begins at column 1
101 | #-------------------------------------------------------------------------
102 | 1
103 | #-------------------------------------------------------------------------
104 | # LIMS[1][3]: and continues until column 20
105 | #-------------------------------------------------------------------------
106 | 20
107 | #-------------------------------------------------------------------------
108 | # TSURF[1]: Temperature of surface 1
109 | #-------------------------------------------------------------------------
110 | 300
111 | #-------------------------------------------------------------------------
112 | # ISURF[2]: Direction of surface 2 normal is in the negative y direction
113 | #-------------------------------------------------------------------------
114 | 2
115 | #-------------------------------------------------------------------------
116 | # LIMS[2][1]: Surface 2 lies along lower boundary of this row
117 | #-------------------------------------------------------------------------
118 | 201
119 | #-------------------------------------------------------------------------
120 | # LIMS[2][2]: Surface 2 begins at column 1
121 | #-------------------------------------------------------------------------
122 | 1
123 | #-------------------------------------------------------------------------
124 | # LIMS[2][3]: and continues until column 20
```

```
125 |#-------------------------------------------------------------------
126 |20
127 |#-------------------------------------------------------------------
128 |# TSURF[2]: Temperature of surface 2
129 |#-------------------------------------------------------------------
130 |30000
131 |#-------------------------------------------------------------------
132 |# NIS: The number of DTM time steps between samplings
133 |#-------------------------------------------------------------------
134 |2
135 |#-------------------------------------------------------------------
136 |# NSP: The number of samples between prints
137 |#-------------------------------------------------------------------
138 |10
139 |#-------------------------------------------------------------------
140 |# NPS: The number of prints until assumed start of steady flow
141 |#-------------------------------------------------------------------
142 |30
143 |#-------------------------------------------------------------------
144 |# NPT: The total number of prints
145 |#-------------------------------------------------------------------
146 |50000
147 |#-------------------------------------------------------------------
148 |# Y value for which output will be collected in the LOG FILE
149 |#-------------------------------------------------------------------
150 |0.00584
151 |#-------------------------------------------------------------------
152 |# Row Number Containing Molecule to Track
153 |#-------------------------------------------------------------------
154 |100
155 |#-------------------------------------------------------------------
156 |# Step size for molecule position output to file
157 |# i.e. if next data line is 10 then position information will be
158 |# written to the file every 10 time steps
159 |# Use 1 to output a position after every time step
160 |#-------------------------------------------------------------------
161 |10
162 |#-------------------------------------------------------------------
163 |# Number of Rows for which Output is Desired.
164 |# If this value equals or exceeds the total number of rows then data
165 |# will be output for all rows.
166 |#-------------------------------------------------------------------
167 |10
168 |#-------------------------------------------------------------------
169 |# Row Numbers to Output.
170 |# Required if previous data line is greater than zero and less than the
171 |# total number of rows.
172 |#-------------------------------------------------------------------
173 |20
174 |40
175 |50
176 |60
177 |80
178 |100
179 |120
180 |140
181 |160
182 |180
```