A&AE 590D Molecular Gas Dynamics

Homework 6: Sampling from a Prescribed Distribution

Due: 11/16/06

1) The distribution function of the normal velocity component of the molecules leaving a diffuse wall has the following form:

\[ f(v_n) = 2\beta_w^2 v_n \exp(-\beta_w^2 v_n^2) \]

where \( \beta_w = \frac{1}{2RT_w} \), and \( T_w \) is the wall temperature. Write a program that uses the inverse cumulative distribution function method to sample normal component of velocity of diffusely reflected molecules. Sample 1,000,000 velocity components, plot the histogram and compare it to the distribution function.

2) The distribution function of the rotational energy \( \epsilon \) of nonlinear polyatomic molecules in equilibrium at a temperature \( T \) has the following form (called Maxwell-Boltzmann distribution):

\[ f(\epsilon) = \frac{1}{\Gamma(3/2)} \left( \frac{\epsilon}{kT} \right)^{3/2} \exp\left(-\frac{\epsilon}{kT}\right) \]

where \( \Gamma \) is the gamma-function, \( \Gamma(3/2) = \frac{\sqrt{\pi}}{2} \). Write a program that uses acceptance-rejection method to sample rotational energies for 1,000,000 nitrogen molecules at room temperature. Plot the histogram and compare it to the distribution function.

3) (Bonus) Implement the majorant frequency (MF) scheme of DSMC method in \texttt{dsmceq} program. Compare the collision rates for NTC and MF schemes.