PHYS3071/7073 - Due Friday, 16th of May, 2014 by 11am

Assignment 9 —- Maxwell-Boltzmann distribution

Theory

The Maxwell-Boltzmann speed distribution yields the integral

$$g(v_{\max}) = 4\pi \left(\frac{m}{2\pi k_{\mathrm{B}} T}\right)^{3/2} \int_0^{v_{\max}} \mathrm{e}^{-mv^2/2k_{\mathrm{B}}T} v^2 dv \tag{1}$$

for the fraction of the molecules at temperature T with mass m having speed less than $v_{\max}$, where k_{B} is Boltzmann's constant.

1 Problem 1/5

Boltzmann's constant has the value $k_B = 1.38 \cdot 10^{-23}\,\mathrm{m}^2\,\mathrm{kg/s}^2\,\mathrm{K}$, which is very small. This can cause problems in the numerical integration, so it is better that (1) be expressed in dimensionless units. Rescale (1) to use $\sqrt{2k_{\mathrm{B}}T/m}$ as the unit of velocity so that you end up with a new function $\bar{g}$ of the dimensionless velocity $\bar{v}_{\max}$ which takes the form,

$$\bar{g}(\bar{v}_{\max}) := g\left(\bar{v}_{\max}\sqrt{2k_{\mathrm{B}}T/m}\right) = \alpha \int_0^{\bar{v}_{\max}} \mathrm{e}^{-\beta \bar{v}^2} \bar{v}^2 d\bar{v}. \tag{2}$$

where α and β are dimensionless quantities. Put the values you obtained for α and β (in exact closed form, not numeric decimal form) in a text file named

`as09-analysis-surname-studentid.txt`

Practice

Recall that in worksheets 16 and 17, you learned how to integrate continuous functions such as polynomials, exponentials and trigonometric functions numerically using the Trapezoidal rule via the following formula,

- **Trapezoidal Rule**

$$\int_a^b f(x)dx \approx \frac{h}{2}\left[f_0 + 2\left(\sum_{k=1}^{N-1} f_k\right) + f_N\right] \pm \frac{(b-a)^3\,|f''(M)|}{12N^2}, \tag{3}$$

where $|f''(M)|$ refers to the maximum value of the second derivative of f on the interval $[a, b]$. In worksheet 17 we used the analytic error terms to compute the number of intervals N needed to numerically evaluate integrals to within given accuracy. In general, though, it may not be possible to solve for the number of intervals beforehand. In such cases, we can instead compute the error after the integration to determine whether N was sufficiently large; if the error is too large, then we double N and try again.

When estimating the error after the integration, we set $|f''(M)| := \max|f''(x_k)|$, that is, at each point in the integral we evaluate the second derivative of f in order to keep track of the largest value we have seen so far so that at the end we have an estimate for $|f''(M)|$ to use for the error.

2 Problem 2/5

Write a C program that takes as input

- the highest velocity, $\bar{v}_{\max}$ (in the dimensionless units specified above); and
- the desired accuracy, E;

and then does the following. Starting with $N = 2$, it evaluates the integral in equation (2) using the trapezoid rule, as well as the estimated error given in (3) where $|f''(M)|$ is obtained by evaluating the second derivative of the integrand as well as the integrand at each point in the interval (i.e., $0, \frac{b}{N}, \frac{2b}{N}, \ldots, b$) and setting $|f''(M)|$ to the maximum observed value of the second derivative. If the estimated error is not less than the desired accuracy, then keep doubling N and repeating this procedure until it is.

The output of the program (printed to the screen) should be a nicely formatted table with one line for each value of N used by your integration code containing the following information:

- the number of intervals, N;
- the estimated value of the integral, $\bar{g}(\bar{v}_{\max})$; and
- the estimated error

In addition to the table, the program should at the end also output the converged value of the integral and the number of intervals used to obtain it. When outputting the tables use a C format string to create fixed-width columns and put appropriate labels at the top.

Hint: You can test your program using the following data point:

- $\bar{g}(0.75) = 0.228957330$;

3 Problem 3/5

Take the program you wrote in Problem 2 and run it on the values:

1. $\bar{v}_{\max} = 1$
2. $\bar{v}_{\max} = 2$
3. $\bar{v}_{\max} = 3$

with $E = 10^{-8}$. For each of these outputs, copy and paste the output of your program into

`as09-output-surname-studentid.txt`

4 Problem 4/5 (Advanced)

We now want to integrate the Maxwell-Boltzmann distribution up to $v = \infty$. In order to do this, we will apply the variable transformation $v = \frac{1}{t} - 1$ to eq. 2. This will allow us to do the integration within finite limits while at the same time ensuring that the modified function does not become infinite within the integration limits. Add a description of the new function that you get and the integration intervals to the file

`as09-analysis-surname-studentid.txt`

Also create a properly labeled plot of the modified function with name

`as09-plot-surname-studentid.ps`

5 Problem 5/5 (Advanced)

Write a program that can integrate the new function with the midpoint method. The input should consist now only of the stepsize Δt. Once the integration is finished, your program should print out the estimated value for the integral of the Maxwell-Boltzmann distribution.

Submission

To submit your assignment copy the program you wrote for problem 2 to `as09-problem2-surname-studentid.c` and copy the program you wrote for problem 5 to `as09-problem5-surname-studentid.c`. The full set of files you will have when you are done is:

- `as09-problem2-surname-studentid.c`
- `as09-problem5-surname-studentid.c`
- `as09-analysis-surname-studentid.txt`
- `as09-output-surname-studentid.txt`
- `as09-plot-surname-studentid.ps`

To submit your assignment, upload the above files to your directory, eg. s1234567/as09/. Name the new directory `as09`. Upload the C programs and the text file with COURSENUMBER AS09 SURNAME STUDENTID (case doesn't matter) at the top. Your postscript figure should have the same information in its title, i.e. use `set title <COURSENUMBER> AS09 <SURNAME> <STUDENTID>`.

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Grading Sheet – Assignment 9 Maxwell-Boltzmann distribution

A: /30% **Function**: Does the program run and produce the correct output?

C: /5% **Usability**: Is the program easy to use? Are the input requirements and output formatting easy to understand?

D: /5% **Readability**: Is the program easy to read and comprehend? Is it well-commented? If the code is sufficiently complex, has it been broken up into manageable subroutines, each of which is well-documented?

E: /10% **Efficiency**: Does the program run efficiently? Is the coding clunky or unnecessarily complicated?

B: /10% **Output/plots**: Is the program output correct ? Do the plots clearly convey the results? Does each plot have an appropriate title? Are the axes and the plot items clearly labeled?

F: /20% **Analysis**: Were correct answers given to the questions asked in the assignment, and was the process used to obtain them reasonable and clearly explained?

G: /20% **Advanced part**: Grading for this part follows the same rules as detailed under points A to F.

Total Points: | /100 |