MAS.864: Derivation of 2D Boltzmann Distribution

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From the Kinetic Theory of gases, the general form of the probability density function of the velocity component of a gas particle is of the form

$$p(v_i) = Ae^{-Bv_i^2}. \tag{1}$$

Since we are in 2 dimensions, the speed of a particle is

$$v = \sqrt{v_x^2 + v_y^2}. \tag{2}$$

with differential element $vdvd\theta$. Integrating θ from 0 to 2π, we can see that the speed probability density function is

$$p(v) = 2\pi v A^2 e^{-Bv_i^2}. \tag{3}$$

Using normalization, and the standard integral

$$\int_0^\infty xe^{-Bx^2} = \frac{1}{2B}, \tag{4}$$

One can show that

$$A = \sqrt{\frac{B}{\pi}}. \tag{5}$$

Hence, the only free parameter to be determined is B, which will now be pursued

Given that the average kinetic energy of a particle with 2 degrees of freedom (in the 2-dimensional case for a spherical particle) is kT where k is the Boltzmann constant and T the thermodynamic temperature, it follows that

$$\overline{\tfrac{1}{2}mv^2} = \int_0^\infty \frac{1}{2}mv^2 \; p(v) = kT. \tag{6}$$

Integrating above equation and solving for B, one can determine that $A = \sqrt{\frac{m}{2kT\pi}}$ and $B = \frac{m}{2kT}$. This leads to the probability density function to be

$$p(v) = \frac{m}{kT} \; ve^{-\frac{m}{2kT}v^2} \tag{7}$$

$$= \frac{v}{\sigma^2}e^{-\frac{v^2}{2\sigma^2}} \tag{8}$$

for $\sigma = \sqrt{\frac{kT}{m}}$ where σ is equal to the standard deviation of the x and y-velocity Gaussian distribution. Hence it is useful to express the Boltzmann distribution function of speed in this form.

Finally, the general form of a Boltzmann density function

$$p(v) = \gamma \, \frac{v^{\alpha}}{\sigma^{\beta}} e^{-\frac{v^2}{2\sigma}} \tag{9}$$

will be used for non-linear fitting of the simulation data. It will be shown that $\alpha = 1$, $\beta = 2$ and $\gamma = 1$, matching the analytically derived Boltzmann density function in 2 dimensions.

The plots below refer to the x and y-velocity histograms and their corresponding Gaussian fit. The last plot corresponds to the Boltzmann distribution histogram. The yellow curve is the 3D fit, the red curve is the analytical fit, while the blue curve is the non-linear fit with least-square determined $\alpha = 1.00926482$, $\beta = 2.03568257$ and $\gamma = 1.0649113$.

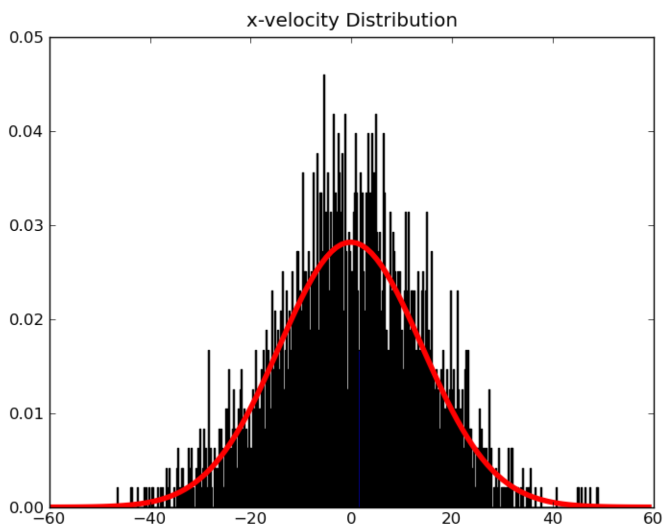

Figure 1: Normalized distribution of x-velocities of 2500 particles

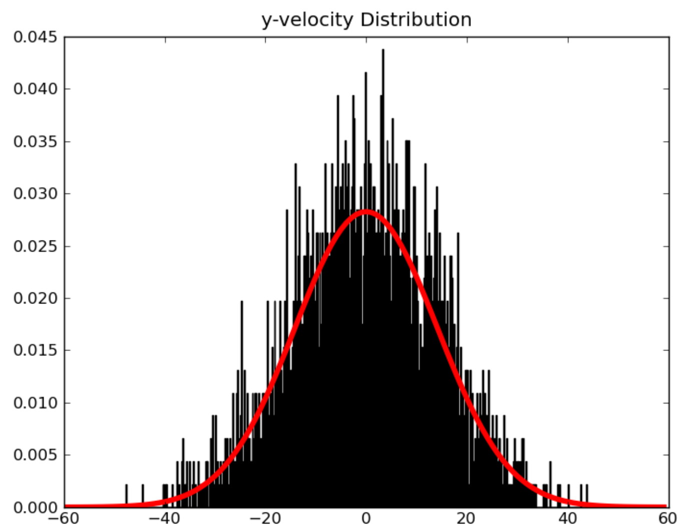

Figure 2: Normalized distribution of y-velocities of 2500 particles

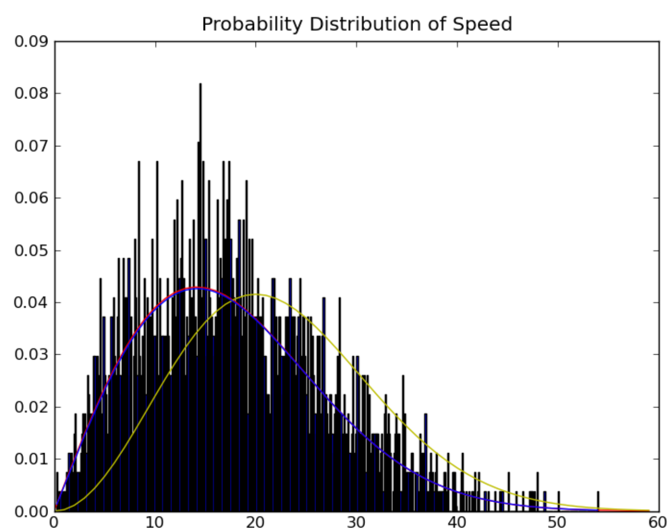

Figure 3: Normalized distribution of speeds of 2500 particles