Generating random deviates from the Maxwell flux distribution

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The Maxwell flux distribution of velocities reads

$$f(v_x, v_y, v_z)\, dv_x\, dv_y\, dv_z = \frac{2}{\pi} e^{-v_x^2 - v_y^2 - v_z^2} v_z \; dv_x\, dv_y\, dv_z, \tag{1}$$

with $0 < v_z < \infty$ and $-\infty < v_x, v_y < \infty$. Here velocities are scaled to the thermal velocity $v_T = \sqrt{2kT/m}$ and the distribution is normalized to 1. Going to cylindrical coordinates (v_ρ, ϕ, v_z) we get

$$\frac{2}{\pi} e^{-v_\rho^2 - v_z^2} v_z\, v_\rho\, dv_\rho\, d\phi\, dv_z = \left[2\, e^{-v_z^2} v_z\, dv_z\right] \left[2\, e^{-v_\rho^2} v_\rho\, dv_\rho\right] \left[\frac{1}{2\pi}\, d\phi\right],$$

thus v_ρ and v_z are identically distributed according to $g(x) = 2xe^{-x^2}$ and ϕ is uniformly distributed in $[0, 2\pi)$.

For $g(x)$ we have

- Normalization: $\int_0^\infty g(x)\, dx = 1$.
- CDF: $G(x) = \int_0^x g(x')\, dx' = 1 - e^{-x^2}$.
- Inverted CDF: $G(x) = z \Rightarrow x = \sqrt{-\log(1 - z)}$.

To create random velocities with the Maxwell distr. we first create three uniform deviates (u_1, u_2, u_3) in $(0, 1)$. Then

$$\begin{aligned} v_z &= \sqrt{-\log u_1} \\ v_y &= \sqrt{-\log u_2}\, \sin(2\pi u_3) \\ v_x &= \sqrt{-\log u_2}\, \cos(2\pi u_3) \end{aligned}$$

If we just need the magnitude of the velocity, then only (u_1, u_2) are required

$$v = \sqrt{v_x^2 + v_y^2 + v_z^2} = \sqrt{-\log u_1 u_2}$$