INVESTIGATING VELOCITY MOMENTS IN ARBITRARY DIMENSIONAL SYSTEMS

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Abstract

The kinetic theory of gases is an important element of undergraduate training in various engineering and scientific fields. This article presents a general derivation of the moments of the Maxwell-Boltzmann velocity distribution for arbitrary dimension. Numerical simulations of hard hypersphere collisions are performed to test the theoretical predictions. Good agreement is found. Such activities expose students to special functions, numerical simulation methods and graphics software.

Introduction

Students in engineering and science need to understand the relationship between microscopic molecular motion and macroscopic properties. The kinetic theory of gases [1] makes this connection by relating macroscopic properties such as the temperature to the average of the square of the velocities of individual particles. In D dimensions the kinetic energy, ½ m$<V^2>$, is given as

$$\tfrac{1}{2} m<V^2> = \tfrac{1}{2} D\, k_B T \quad (1)$$

Here, m is the mass of the particles, $<V^2>$, is the average of the square of their velocities, k_B is Boltzmann's constant and T is the absolute temperature. The right side of Eq. 1 follows from the law of equipartition [1]. Each degree of freedom contributes one factor of ½ $k_B T$ to the energy and there are D total translational degrees of freedom for unstructured hard hyperspheres in D dimensions. In this article we employ reduced units for which $m/k_B T = 1$.

The velocities follow the Maxwell-Boltzmann probability distribution function. This distribution function is essentially a Gaussian distribution. The D-dimensional Gaussian distribution, P(V), is given by

$$P(V) = [D / (2\pi<V^2>)]^{D/2} \exp(- DV^2 /(2<V^2>)) \quad (2)$$

P(V) must obey the normalization condition for probabilities:

$$1 = \int_{-\infty}^{\infty} \ldots \int_{-\infty}^{\infty} P(V)\, \mathbf{dV} \quad (3)$$

where **dV** in Eq. 3 is the appropriate volume element in D-dimensional velocity space.

In two dimensions (D=2) for example, the volume element in Cartesian coordinates is dVx dVy. Since the velocities have angular symmetry, polar coordinates can be employed to reduce the integral over two separate components, Vx and Vy, to a single integral. The volume element in polar coordinates is **dV** = dθ VdV.

Then Eq. 3 becomes

$$1 = [1/(\pi<V^2>)] \int_0^{\infty} \int_0^{2\pi} \exp(-V^2/(<V^2>))\, d\theta\, V dV \quad (4)$$

The right hand side of Eq. 4 evaluates to 1 as expected.

According to Eq.1, in D dimensions,

$$<V^2> = D \quad (5)$$

The general equation for the average value of the Q - th moment of velocity, $<V^Q>$, is given by

$$\langle V^Q \rangle = \int_{-\infty}^{\infty} \ldots \int_{-\infty}^{\infty} V^Q \, P(V) \, \mathbf{dV} \qquad (6)$$

To transform this general case which involves D component integrals to a single integral over the magnitude of **V**, |**V**|, one needs to relate the Cartesian coordinates of **V** to its D dimensional spherical coordinates involving |**V**| and the D - 1 angles $\theta_1\ \theta_2 \ldots \theta_{D-1}$. Alternatively, one can reformulate the integration procedure as integrating over the surface area of a D-dimensional hypersphere, Ω_D. To do this we change the expression given in Tiglias and Bishop [2] in R space to V space, to find that

$$\Omega_D = 2\,\pi^{D/2}\, V^{D-1} / \Gamma(D/2) \qquad (7)$$

where, Γ is the Gamma function [3]

$$\Gamma(x) = \int_0^{\infty} t^{x-1} \exp(-t)\, dt \qquad (8)$$

Thus, the general equation for the Q - th moment can be recast as

$$\langle V^Q \rangle = \int_0^{\infty} V^Q \, P(V)\, \Omega_D \, dV \qquad (9)$$

or

$$\langle V^Q \rangle = \{2\pi^{D/2} / \Gamma(D/2)\}\,[D / (2\pi\langle V^2\rangle)]^{D/2} \int_0^{\infty} V^{Q+D-1} \exp(-DV^2 / (2\langle V^2\rangle))\, dV \qquad (10)$$

Using Eq. 5, this simplifies to

$$\langle V^Q \rangle = [2^{1-D/2} / \Gamma(D/2)] \int_0^{\infty} V^{Q+D-1} \exp(-V^2/2)\, dV \qquad (11)$$

If we set $Z = V^2/2$, Eq. 11 reduces to

$$\langle V^Q \rangle = [2^{Q/2} / \Gamma(D/2)] \int_0^{\infty} Z^{(Q+D)/2-1} \exp(Z)\, dZ \qquad (12)$$

which becomes

$$\langle V^Q \rangle = 2^{Q/2}\ \Gamma((Q+D)/2)\ /\ \Gamma(D/2) \qquad (13)$$

Eq. 13 is the generalized D-dimensional Q-th moment which will be compared with simulation results.

When Q = 2, one finds that

$$\langle V^2 \rangle = 2\,\Gamma((2+D)/2) / \Gamma(D/2) \qquad (14)$$

However, one of the properties [3] of the Gamma function is that Γ(1 + X) = X Γ(X). It then follows that

$$\Gamma((2+D)/2) = \Gamma(1+D/2) = (D/2)\,\Gamma(D/2) \qquad (15)$$

and Eq.5 is obtained.

Similarly, when Q = 4, 6 and 8 we find that

$$\langle V^4 \rangle = (D+2)\,D \qquad (16)$$

$$\langle V^6 \rangle = (D+4)(D+2)\,D \qquad (17)$$

and

$$\langle V^8 \rangle = (D+6)(D+4)(D+2)\,D \qquad (18)$$

The numerical values for these moments when D = 2 through 5 are listed in Table I.

Table I. Theoretical values of the moments in different dimensions

D	$<V^2>$	$<V^4>$	$<V^6>$	$<V^8>$
2	2	8	48	384
3	3	15	105	945
4	4	24	192	1920
5	5	35	315	3465

Computer Simulation

We have developed an independent study project for a simulation and modeling course which tests Eq.13 for D = 2 through 5 dimensions by computing the moments of the velocity distribution of hard hyperspheres. Detailed discussions of the properties of hard particle systems are available in the literature [4,5,6]. These sources also include sample codes.

We first consider a two dimensional system with N disks at a density ρ. These parameters determine the side length of a box containing the disks

$$L = (N / \rho)^{1/2} \quad (19)$$

Each disk is given an initial position and velocity. Let two disks, i and j, with a diameter of one in our reduced system of units, have positions $\mathbf{r}i$ and $\mathbf{r}j$ and velocities $\mathbf{v}i$ and $\mathbf{v}j$ at time t. If these disks are to collide at time t + tij, e.g. be tangent, then

$$| \mathbf{r}ij(t+tij)| = |\mathbf{r}ij + \mathbf{v}ij * tij| = 1 \quad (20)$$

where $\mathbf{r}ij = \mathbf{r}i - \mathbf{r}j$ and $\mathbf{v}ij = \mathbf{v}i - \mathbf{v}j$. Define $bij = \mathbf{r}ij \cdot \mathbf{v}ij$ and then Eq. 20 becomes

$$vij^2\, tij^2 + 2bij\, tij + rij^2 - 1 = 0 \quad (21)$$

This is a quadratic equation in tij. If bij > 0 the disks are moving away from each other and will not collide. The discriminant cannot be negative or the equation will have complex roots. Taking the smaller of the two roots, one finds that

$$tij = [- bij - (bij^2 - vij^2 (rij^2 -1))^{1/2}] /vij^2 \quad (22)$$

Then the tijs for all the possible pairs need to be computed. This is an $O(N^2)$ calculation if done directly inside two nested loops over i and j. We have utilized this approach for simplicity. The smallest tij value is selected and all particles are moved for that time. The velocities of the colliding pair then change. We assume perfectly elastic collisions for which the kinetic energy and linear momentum are conserved. Then

$$\mathbf{v}i \text{ (after)} = \mathbf{v}i \text{ (before)} + d\mathbf{v}i \quad (23a)$$

and

$$\mathbf{vj} \text{ (after)} = \mathbf{vj} \text{ (before)} - d\mathbf{v}i \quad (23b)$$

where

$$d\mathbf{v}i = - bij\, \mathbf{r}ij \quad (24)$$

bij is evaluated at the moment of impact.

Now the tijs of all particles which would have collided with particle i or j need to be updated. After this procedure a new shortest tij is found and the process repeated. In this manner the two dimensional hard disks are moved. We have selected a ρ value of 0.2. A total of 1,000,000 collisions are followed and 500,000 are discarded to allow for equilibration. Data is gathered every 1,000 collisions and the mean and standard deviation of the 500 samples are obtained via standard methods [7]. It is simple to extend this analysis to higher dimensions since all the above equations are cast in terms of vectors. Figure 1 illustrates the locations of 64 three dimensional spheres at a density of 0.2. The left panel contains a snapshot of the starting configuration whereas the right panel is a snapshot of the last configuration.

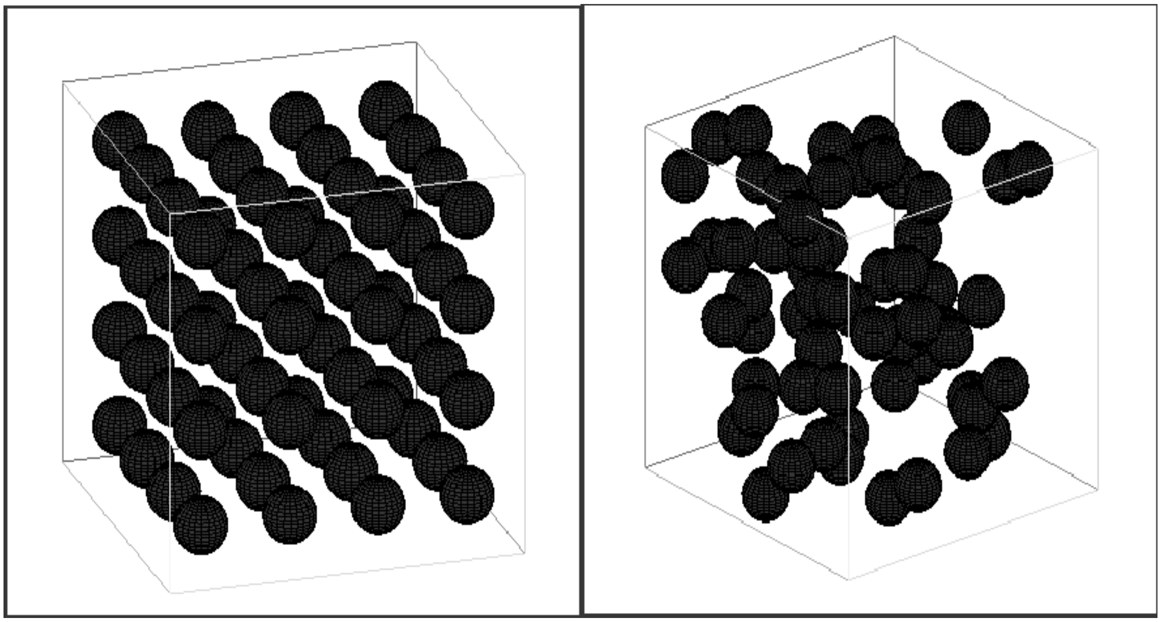

Figure 1: Snapshots of the initial and final configurations when N=64, Density=0.2, with 100,000 collisions discarding the first 50,000.

Table II. Values of the velocity moments in different dimensions obtained by simulation

D	N	$\langle V^2 \rangle$	$\langle V^4 \rangle$	$\langle V^6 \rangle$	$\langle V^8 \rangle$
2	625	1.993±0.004	7.969±0.021	47.864±0.266	383.688±0.446
3	512	2.983±0.006	14.748±0.036	101.080±0.481	880.922±8.764
4	625	3.994±0.008	23.925±0.054	190.355±0.699	1884.22±13.15
5	243	4.996±0.010	34.905±0.083	312.429±1.362	3401.66±28.72

The program was coded in C++. The simulation results are contained in Table II.

There is generally good agreement between these values and the theoretical predictions in Table I. The differences from the theoretical values depend upon the number of hyperspheres, the number of collisions, and the magnitude of the quantity studied.

Conclusions

We have presented a general derivation and performed computer simulations of the average moments of the velocity of hard particle systems in two to five dimensions. The agreement between the theoretical predictions and the computer results for the second, fourth, sixth and eighth moment of velocity depends upon a number of factors. Having students numerically compute these moments exposes them to important ideas in kinetic theory, computer modeling, computer programming and statistical tools which will be of great use in their future careers. Snapshots generated with the Maple software package reveal the random arrangement of particles after a sufficient number of collisions and further enhance student understanding. This project demonstrates the key elements of simulation and the impact of statistical fluctuations.

Appendix: The Manhattan College Undergraduate Research Program

Manhattan College has a long tradition of involving undergraduates in research and was one of the original members of the Oberlin 50 [8]. This is a group of undergraduate institutions whose students have produced many PhDs in engineering and science. At Manhattan College, students can elect to take an independent study course for 3 credits during the academic year. In addition, the College provides grant support to the students for 10 weeks of work during the summer. I have personally recruited the students from my junior level course in Systems Programming. Previously published articles in this journal by Manhattan College student co-authors are a very effective recruitment tool. The students have also presented their results at a variety of undergraduate research conferences including the Hudson River Undergraduate Mathematics Conference and the Spuyten Duyvil Undergraduate Mathematics Conference.

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8. The Oberlin 50 institutions are: Albion College, Alma College, Amherst College, Antioch University, Barnard College, Bates College, Beloit College, Bowdoin College, Bryn Mawr College, Bucknell University, Carleton College, Colgate University, Colorado College, Davidson College, Denison University, DePauw University, Earlham College, Franklin and Marshall College, Grinnell College, Hamilton College, Hampton University, Harvey Mudd College, Haverford College, College of the Holy Cross, Hope College, Kalamazoo College, Kenyon College, Lafayette College, Macalester College, Manhattan College, Middlebury College, Mount Holyoke College, Oberlin College, Occidental College, Ohio Wesleyan University, Pomona College, Reed College, Smith College, St. Olaf College, Swarthmore College, Trinity College (CT), Union College (NY), Vassar College, Wabash College, Wellesley College, Wesleyan University, Wheaton College (IL), Whitman College, Williams College, and College of Wooster.

Biographical Information

Abraham Asfaw is currently studying for a B.S.E. in Electrical Engineering at Manhattan College.

Marvin Bishop is a Professor in the Department of Mathematics and Computer Science at Manhattan College. He received his Ph. D. from Columbia University, his M.S. from New York University and his B.S. from the City College of New York. His research interests include simulation and modeling and parallel processing.