Computer simulation of a two-dimensional ideal gas: a simple molecular dynamics method for teaching purposes

Eur. J. Phys. 6 (1985) 148–153. Printed in Northern Ireland

Computer simulation of a two-dimensional ideal gas: a simple molecular dynamics method for teaching purposes

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Received 24 July 1984

Abstract A simple two-dimensional model of an ideal gas is described in order to study the time evolution of speed distribution in the framework of newtonian mechanics. The results of a computer simulation of a system of 16 particles are shown. The approach to equilibrium is followed by observing changes in the experimentally obtained values of Boltzmann's H. An example of a possible way to use this simulation program in an introductory physics course is also given.

Riassunto Questo lavoro descrive un semplice modello bidimensionale di gas perfetto, allo scopo di studiare la evoluzione temporale della distribuzione delle velocità, nell' ipotesi della dinamica Newtoniana. Il modello è utilizzato per una 'computer simulation' a scopo didattico, e sono descritti in dettaglio i risultati ottenuti con un sistema di 16 particelle. L'approssimarsi all'equilibrio del sistema è seguito osservando la evoluzione dell' H di Boltzmann. E' inoltre descritta una possibile utilizzazione didattica del programma di simulazione in un corso introduttivo di fisica per studenti universitari.

1. Introduction

The understanding of microscopic disordered motion in gases is usually a difficult problem for most science students following typical introductory physics courses. The Maxwell–Boltzmann distribution function is usually presented as merely an empirical formula. In fact the analytical approach connecting the results of the kinetic theory of gases and the dynamic behaviour of simple systems (e.g. hard spheres colliding elastically) is not straightforward.

Mechanical apparatus is often used to illustrate the behaviour of molecules in gases, but the need to continuously supply energy to the system can introduce misconceptions about the meaining of an isolated system (Iona and Hastings 1970, Eaton *et al* 1979). The use of computer simulations in the microphysical area is, however, more interesting, since these simulations can supply 'experimental' support for physical theories. Many interesting computer simulations of ideal gases have been published for teaching purposes. Most of these use totally or partially stochastic approaches, assuming different probability distributions for collisions between pairs of molecules and 'scattering generators' (Novak and Bortz 1970, Eger and Kress 1982, Ftáčnik *et al* 1983, Bonomo and Riggi 1984).

Well structured teaching courses should cover all possible links between different fields of physics, yet the associations between dynamics and thermodynamics and between dynamics and statistical physics are topics which are usually insufficiently related in introductory physics books. Sauer (1981) provided evidence for the pedagogical value of a computer simulation demonstrating disordered motion of gases in the framework of newtonian mechanics. He also used a Monte-Carlo procedure for the simulation of statistical ensembles and compared the results of the two methods. He proposed a one-dimensional model in which neighbouring particles had different masses in order to allow for thermalisation.

Many studies in molecular dynamics have already used computer simulations to study equilibrium and nonequilibrium properties of models of molecular

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systems (Alder and Wainwright 1959, 1963, Erpenbeck and Wood 1977). These studies solve numerically the equations of motion for a many-bodied system and follow the trajectories of a few hundred particles. To study systems containing as many as several hundred interacting particles, high speed computers with a large memory capacity are required.

The characteristics and the versatility of personal computers have been evaluated as satisfactory and effective for educational purposes. The implementation of a molecular dynamics calculation on a personal computer requires not only a reduction of the number of particles that can be handled but also a simplification of the numerical analysis, as well as an evaluation of the appropriate boundary conditions in order to have small systems representing macroscopic systems as closely as possible.

In this paper we discuss a model simulating a two-dimensional gas. Hard-core interaction is assumed and a molecular dynamics method is used. By starting from different initial conditions a computer simulation of the development of speed distribution as it approaches a Maxwell–Boltzmann distribution is shown for systems containing a low number of particles. The changes in the experimentally determined values of Boltzmann's constant H are also shown in order to study the approach to equilibrium. The program has been written in BASIC and will be described in detail. The hardware used consists of the Apple II Europlus (64 K). An example of a possible way to use this software in an introductory physics course will be also shown.

2. Model and computer simulation

The system studied consists of N identical two-dimensional hard-sphere particles (hard discs) contained in a two-dimensional 'volume' V. We assume hard-core interaction: $u(r)=0$ for $r>\sigma$ and $u(r)=\infty$ for $r<\sigma$, where r is the separation of the centres of a pair of particles and σ is the collision diameter (in this case the diameter D of the discs). Given the initial positions and velocities of the particles and having stated the boundary conditions, the future behaviour of the system is determined.

In order to represent a macroscopic system as closely as possible with a small number of particles contained in a volume V we impose periodic boundary conditions, i.e. we imagine space to be filled by indefinite replications of the volume V and its constituent particles. The primary volume V is a box with penetrable walls and the particles are constrained in such a way that their number in the box remains constant. A particle which leaves the box through one wall is caused to re-enter with unchanged velocity through the opposite wall. Consequently particles interact only with other particles.

Molecular dynamic methods (Erpenbeck and Wood 1977) usually apply periodic boundary conditions in such a way that for each particle i at $\boldsymbol{r}_i$, in the primary (one- two- or three-dimensional) cell of edge L, 'image' particles are located at positions $\boldsymbol{r}_i+\boldsymbol{\nu}L$ for all the vectors $\boldsymbol{\nu}$ having integer components $-\infty<\boldsymbol{\nu}_c<\infty$. We used a simplified version of these periodic boundary conditions because of the limitations imposed by the memory capacity and speed of the computer.

2.1. Method

(i) The initial configuration is set up. The machine can calculate exactly, to the number of significant figures carried, the particle trajectories. All the trajectories are straight until two particles collide or one particle crosses a wall.

(ii) For each pair of particles i and j a collision time t_{ij} is calculated ignoring the presence of other particles. Introducing (Erpenbeck and Wood 1977) relative coordinates and velocities

$$\boldsymbol{r}_{ij}=\boldsymbol{r}_i-\boldsymbol{r}_j \qquad \boldsymbol{v}_{ij}=\boldsymbol{v}_i-\boldsymbol{v}_j$$

particles i and j are approaching each other if $\boldsymbol{r}_{ij}\cdot\boldsymbol{v}_{ij}<0$. Otherwise the collision time is defined as infinite

$$t_{ij}=\infty \qquad \text{for } \boldsymbol{r}_{ij}\cdot\boldsymbol{v}_{ij}\geqslant 0.$$

For each pair of particles that are approaching, the collision time is given by the time required to reach a separation of D (where D is the diameter of the particles). But some approaching particles can never reach a separation of D. From simple kinematic considerations it can be shown that this occurs when

$$b_{ij}^2>D^2$$

where

$$b_{ij}^2=r_{ij}^2-[(\boldsymbol{r}_{ij}\cdot\boldsymbol{v}_{ij})/v_{ij}]^2.$$

If this is the case we define $t_{ij}=\infty$.

Finally the collision time is computed

$$t_{ij}=-\frac{1}{v_{ij}}\left(\frac{\boldsymbol{r}_{ij}\cdot\boldsymbol{v}_{ij}}{v_{ij}}+(D^2-b_{ij}^2)^{1/2}\right) \quad \text{for} \quad b_{ij}^2\leqslant D^2.$$

Moreover, each particle i has a time t_i^b at which, in absence of other particles, it would cross a boundary of the primary cell. This boundary crossing time can be calculated from simple kinematic considerations.

(iii) Among all the $N(N-1)/2$ collision times and the N crossing times calculated the minimum value t_m is selected and the phase is advanced to $t+t_m$ using the straight-line trajectory

$$\boldsymbol{r}_i(t+t_m)=\boldsymbol{r}_i(t)+t_m\boldsymbol{v}_i(t) \quad \text{for} \quad i=1,2,\ldots,N$$

(iv) If t_m is given by t_i^b the appropriate coordinate of the particle i is translated by L. If t_m is given by

t_{ij} the post-collision velocities of the particles i and j are computed on the basis of momentum and energy conservations. Consequently

$$\Delta \boldsymbol{v}_i = -\Delta \boldsymbol{v}_j = -\frac{\boldsymbol{r}_{ij}(\boldsymbol{r}_{ij} \cdot \boldsymbol{v}_{ij})}{D^2}$$

and the post-collision velocities are

$$\boldsymbol{v}_i' = \boldsymbol{v}_i + \Delta \boldsymbol{v}_i \qquad \boldsymbol{v}_j' = \boldsymbol{v}_j + \Delta \boldsymbol{v}_j.$$

By iteration of the last three steps the phase can be advanced indefinitely.

Although our method is very simple, it requires a lot of computations for the various steps. Consequently, very few particles can be treated in a reasonable time. A great saving in computing time can be made by defining a table of the collision and the boundary-crossing times.

New t_{ij} and t_i^b are calculated only for particles that just collided or crossed the wall and these values are inserted in the table if they are less than the largest t_{ij} present on the table. All the other t_{ij} and t_i^b are only diminished by the t_m previously computed (Alder and Wainwright 1959).

After each collision between two particles the new speed distribution is calculated (given the cut-off velocity v_c and the width of the interval Δv). An average distribution after a selected number of particle collisions can be plotted and compared with the theoretical Maxwell–Boltzmann distribution. For the two-dimensional case $f(v) \propto v \exp(-v^2/\langle v^2 \rangle)$ where $\langle v^2 \rangle$ denotes the mean quadratic velocity.

In order to have information about the decay of the speed distribution towards the Maxwell–Boltzmann distribution, the program calculates the ratio $n(v)/n_M(v)$ (number of particles in a given speed interval divided by the expected equilibrium number in the same interval). Moreover, it calculates the average M of these ratios on all intervals analysed and the standard deviation. In order to better evaluate the system as it approaches equilibrium, Boltzmann's constant H is evaluated at various points. A discrete form of H is

$$H = \sum_k f(\boldsymbol{v}_k) \lg f(\boldsymbol{v}_k) \delta^3 v_k$$

where $f(\boldsymbol{v}_k)\delta^3 v_k$ is the number of particles in a cell in the neighbourhood of $\boldsymbol{v}_k$ and the sum is over these cells. Taking into account the isotropy in velocity and the two-dimensionality of our velocity space, we obtain

$$H = \sum_0^{v_c} n(v_k) \lg(n(v_k)/\Delta S)$$

where v_c is the cut-off velocity of the simulated distribution, $n(v_k)$ is the number of particles with speed between v_k and $v_k + \Delta v$ and ΔS is the area of the ring (in the v_x—v_y plane) lying between the circles of radius v_k and $v_k + \Delta v$. The approach of the experimental value of H to that calculated if the speeds of the N particles were those expected from the Maxwell–Boltzmann distribution gives a measure of the approach to equilibrium.

3. Results

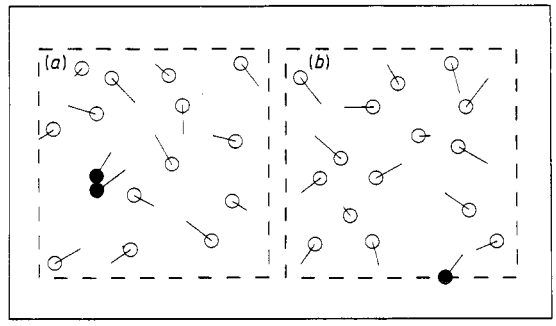
The prepared software follows the time evolution of the spatial distribution as well as of the speed distribution of N equal particles. The characteristics and the initial conditions are chosen from menu and the system evolution is followed in detail until an average of 10–20 collisions per particle have occurred, in order to show how the model is working.

Figure 1 shows a computer display of the position advancement from t to $t + t_m$; figure 1(a) shows a case in which the calculated t_m is a collision time and figure 1(b) shows a case in which the calculated t_m is a boundary crossing time.

Because the relevant part of the system is in momentum space, after a selected number of collisions the speed distributions alone are displayed. Looking at the instantaneous speed distributions it is easily seen that momentum and energy are soon distributed among all the particles in an irregular manner. The comparison of 'snapshots' of velocities taken at different times shows that no reasonable physical information can be drawn about the nature of the distribution function. We need to reduce fluctuations and consequently we need a larger sample.

A larger sample size can be handled, without increasing computing time prohibitively, if we choose to look at the time average distribution. Figure 2 shows different time averages of the speed distributions for the following experiment. Sixteen identical particles were given equal initial velocity magnitude $v_0 = 1$, with a random selection of the

Figure 1 Images of 16 particles in the primary cell and of their trajectories in the time t_m. (a), Two colliding particles (t_m = collision time); (b), a particle crossing the boundary (t_m = crossing time).



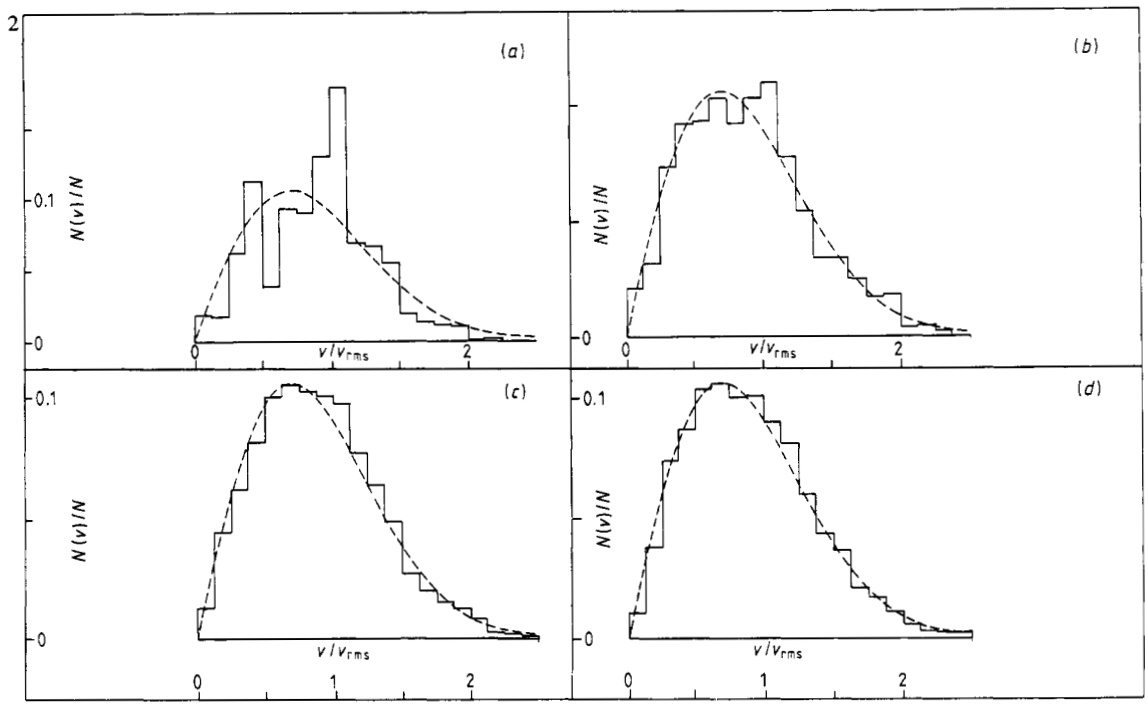


Figure 2 Evolution of the average speed distribution of 16 particles. Initially all particles had equal velocity magnitude $v_0 = 1$ and random directions. The cut-off speed is 2.5 and Δv is 0.125. $N(v)/N$ is the fraction of the total particles for each speed interval. v_{rms} is the root mean square of velocity. $\bar{n}$ is the average number of collisions per particle. Broken curves represent the theoretical Maxwell–Boltzmann distribution. (*a*), $\bar{n} = 10$; (*b*), $\bar{n} = 40$; (*c*), $\bar{n} = 100$; (*d*), $\bar{n} = 200$.

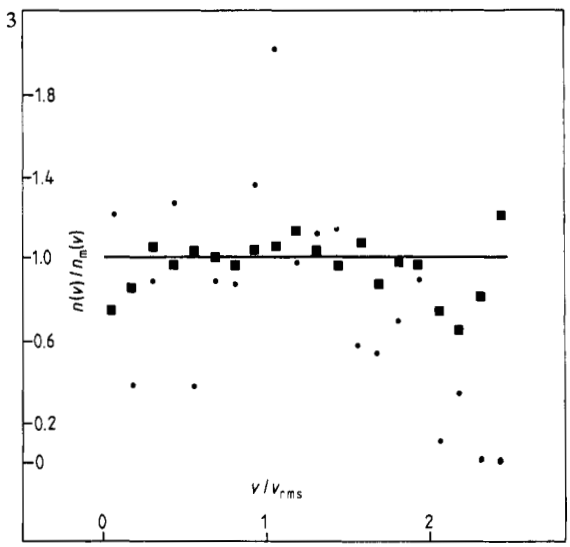


Figure 3 Distribution of the ratio between the number of particles in a given speed interval and the expected equilibrium number in the same interval. ●, values after 80 collisions ($\bar{n} = 10$), $m = 0.79$, $\sigma = 0.57$; ■, values after 1600 collisions ($\bar{n} = 200$), $m = 0.95$, $\sigma = 0.142$.

two direction cosines on the plane; the density was equal to 0.05 with respect to close packing; the initial position was randomly selected on a square box. The different plots refer to averages of different total numbers of collisions (respectively 80, 320, 800 and 1600) and consequently of different numbers of collisions per particle $\bar{n}$. The histograms are the simulated distributions, and the dashed curves represent the Maxwell–Boltzmann distribution. It is clearly shown that the simulated histogram approximates the Maxwell–Boltzmann distribution more closely as $\bar{n}$ increases. In the first two plots an anomaly is evident at $v = 1$, this being a remainder of the initial distribution. The ratios $n(v)/n_M(v)$ have been calculated for two of the simulated distributions reported in figure 2.

Figure 3 is a plot of the distributions of this ratio. It also gives the average values M and the standard deviations. It can easily be seen that the spreading of these ratios is much greater for 80 collisions (10 collisions per particle) than for 1600 collisions (200 collisions per particle).

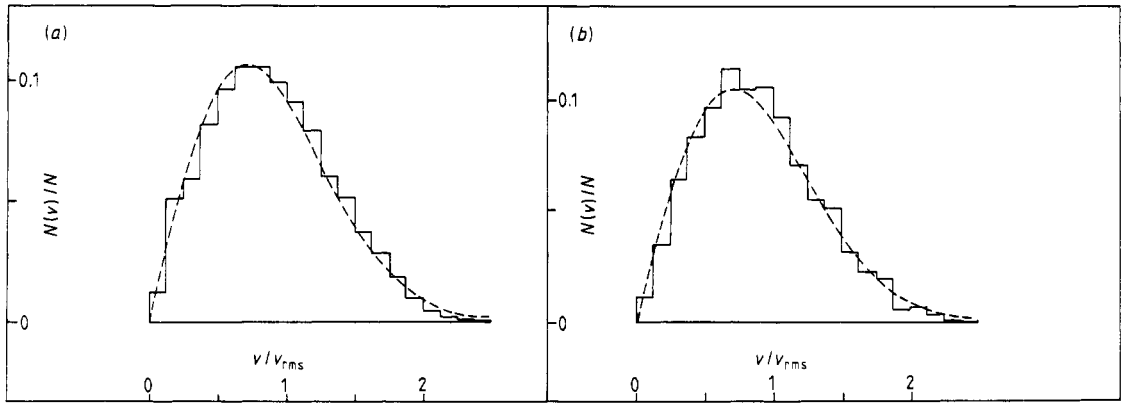


Figure 4 Average distributions of particle speeds among speed intervals for (*a*), $N = 9$, $\bar{n} = 500$; (*b*), $N = 25$; $\bar{n} = 100$.

Different initial conditions, corresponding to the same total energy of the system, have led to the same final result. These observations justify that the macrostate reached after a large number of collisions can be called equilibrium state.

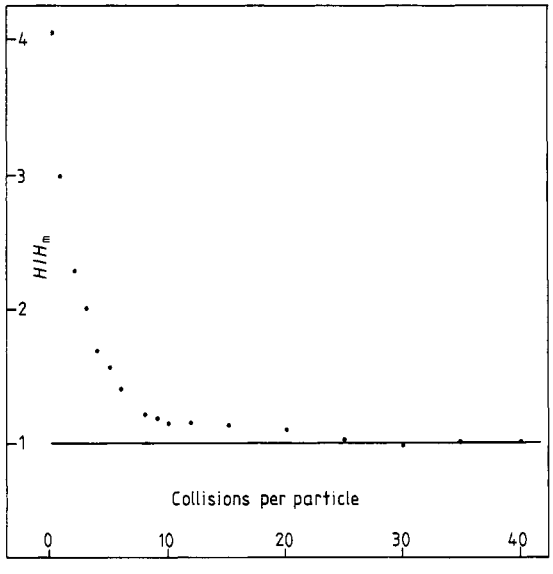
Different numbers of particles have been handled by the program. Figure 4 shows two speed distributions for $N = 9$ and $N = 25$ particle systems. The initial conditions were the same as the experiment described in figure 2. Good fits were obtained with different numbers of collisions per particle ($\bar{n} = 500$ for $N = 9$, and $\bar{n} = 100$ for $N = 25$). In fact, good fits depend on the equilibrium conditions as well as on the total number of particles used to average the speed distributions.

Once the velocity distribution has been determined it is easy to evaluate H. Figure 5 shows the decrease in H as the number of collisions increases, for the same experiment as shown in figure 2. It also shows that H approximates the equilibrium value in 10–15 mean collisions per particle. If we start at this time to average the speed distributions of the particles we can obtain a distribution where the remainder of the initial distribution is reduced.

Figure 6(*a*) shows the speed distribution obtained by averaging from the 81st to the 320th collision for the same experiment as shown in figure 2. Deviations from the theoretical values are nearly randomly distributed but the fit is not yet very good because of the low number of 'snapshots' of particle velocities. In order to reduce these deviations the results of 10 different simulations (concerning equal systems of N particles with the same total energy but different directions of the initial velocities) have been summed and the average distribution has been calculated. The result is shown in figure 6(*b*) and the fit can be considered quite good.

Good fittings can be obtained by averaging the results of different groups of students using appropriate initial conditions.

Figure 5 Ratio between the Boltzmann H and the H equilibrium values H_M plotted against the number of collisions per particle.



4. Conclusions

The educational interest of our computer simulation lies in the possibility of obtaining the Maxwell–Boltzmann distribution using only the framework of newtonian mechanics. The Maxwell–Boltzmann distribution is regarded as a good fit to observation and the computer simulation gives 'experimental' support to the theoretical distribution.

The trial version of the software has been used

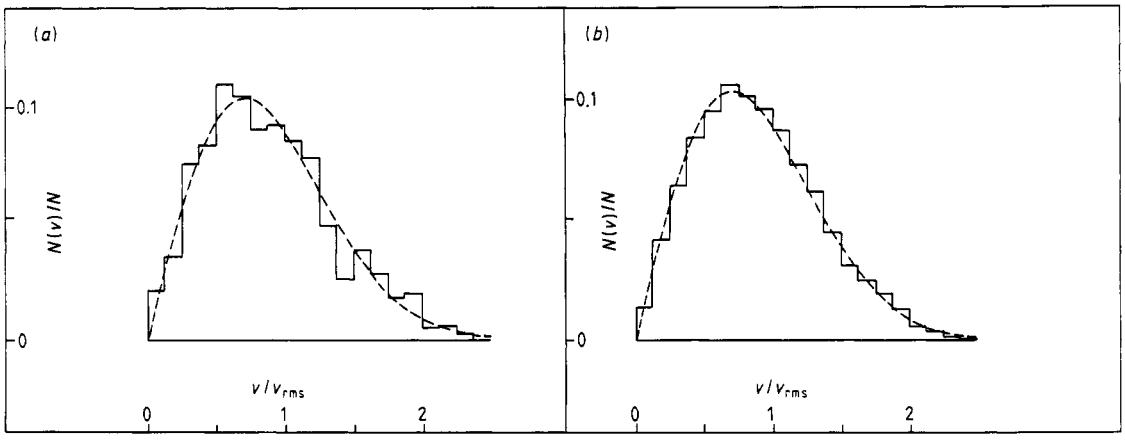


Figure 6 Average distribution of particle speeds among speed intervals for 16 particles. (*a*), The distribution obtained by averaging from the 81st to the 320th collision for the same experiment as shown in figure 2. (*b*), The distribution obtained by averaging 10 simulations like that of (*a*). The 10 systems were identical unless the directions of the initial velocities were different.

by first year science students of our University. Students worked in groups of two or three with the assistance of a tutor, as in their usual laboratory class. A manual is in preparation explaining how the simulation works and how to use the keyboard to enter data. In order to reduce the computing time a BASIC compiler was used for students 'experiments'. In this way one hour is enough to calculate about 300 collisions for the system of 16 particles. Students can carry out a complete simulation and write on file their final distribution. They can successively average their data with that obtained by other students and analyse longer runs using the data previously recorded on file by the teacher or by themselves.

Students have shown a great interest in using the simulation programs and we feel that this kind of computer simulation gives substantial support to the learning process.

Acknowledgment

The present work was supported by Consiglio Nazionale delle Ricerche and MPI local fundings.

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