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A. BRANDT,[1] V. ILYIN,[1] A. SKARBOVIYCHUK[2]

[1] Weizmann Institute of Science
(234, Herzl Str., Rehovot 76100, Israel; e-mail: achi.brandt@weizmann.ac.il, valery.ilyin@weizmann.ac.il)
[2] National University of Food Technology
(68, Volodymyrs'ka Str., Kyiv 01601, Ukraine; e-mail: alex.skarb@gmail.com)

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LARGE SCALE MONTE CARLO SIMULATIONS OF FLUIDS UNDER GRAVITY

A multilevel Monte Carlo method for simulations of fluids under gravity is developed. The approach is based on the Conditional Probability of a state that can be treated as the stochastic equation for the simulated system. The method is illustrated for test cases of a perfect gas and hard-core fluids in one- and two-dimensions, by using model Conditional Probability functions.

Keywords: multilevel, multigrid, Monte Carlo, gravity effect.

Introduction

The Monte Carlo technique is widely used to simulate many-body systems. In the framework of the conventional approach, the current locations of particles are generated with the probability proportional to the Gibbs distribution function [1]. The process is local; one particle is shifted at a time, and this leads to very slow changes of large scale features. Thus, the following inefficiency is inherent to the conventional Monte Carlo method: the larger the scale (that is necessary to approach the thermodynamic limit), the slower the change and the longer (per particle) is the process required to produce new independent features.

In practice, the application of the Monte Carlo technique is restricted to a small, on the macroscopic scale, volume of the system under consideration. For the simulation of a bulk system, the periodic boundary conditions are supposed [1]. It follows from the periodicity conditions that the real system is replaced by a superlattice with the same configurations in each cell. As a result, the fluctuations of the particle number on scales comparable with or larger than the simulation domain are cut off.

The conventional Monte Carlo process leads to reasonable results for many-body systems at high temperatures (when the short-range repulsive contribution to the inter-particle interaction dominates and the correlation length is small). In the neighborhood of a phase change, especially in the critical region, the growth of the correlation size causes a loss of accuracy due to the slowing down of the simulation process [2, 3]. An approach, which allows to overcome this drawback of conventional Monte Carlo methods, consists of a multilevel view of the system [2, 4]. The efficiency of multilevel methods in solving the problems of statistical physics has been shown on examples with sufficiently simple systems [2, 5].

The realistic treatment of critical phenomena is complicated by gravity, which induces a density gradient [6–8]. The method of neutron scattering enables the direct determination of the concentration distribution in the gravitational field near a critical point [8–11]. The density profile changes on the macroscopic (or mesoscopic) scale, and the simultaneous consideration of microscopic features in simulations is difficult because of the large difference in scales. This problem can be avoided in the case of a perfect gas [12, 13]. For more realistic systems, analytical solutions are known only for hard rods under gravity [14–16]. The range of density changes is comparable with the particle size in the case of granular materials [17], and such small systems were successfully studied by simulations [14, 18]. Nevertheless, the small rate of particle exchange between the dense and more dilute regions results in a very slow equilibration [6], i.e., again in the slowing down. Therefore, it is suitable to apply the multilevel Monte Carlo approach to studying the large scale phenomena in many-body systems under gravity.

The aim of the present paper is the development of a general multilevel method for simulations of fluids under gravity. A preliminary version may be found in the Gauss Minerva technical report gmc-15.pdf

1. Multilevel Monte Carlo Method

The Monte Carlo method in the statistical theory is used to evaluate numerically the average $\overline{A}$ of any functional A, defined by:

$$\overline{A} = \int\limits_{\Omega} A(\mathbf{X}) w(\mathbf{X}) d\mathbf{X} \approx \frac{1}{M} \sum_{i=1}^{M} A(\mathbf{X_i}), \tag{1}$$

where $w(\mathbf{X})$ is the probability density of the state $\mathbf{X}$ (the state, or the configuration, is defined by the set of N variables $\mathbf{X} = \{x_1, x_2, ..., x_N\}$) in the configuration space Ω, and *the nodes* $\mathbf{X_i}$ are generated by a random walk in Ω that satisfies detailed balance [1].

The simplest definition of the probability to pass from node $\mathbf{X}$ to $\mathbf{X}'$ in detailed balance is given by:

$$\omega(\mathbf{X} \to \mathbf{X}') = \min\left[1, \frac{w(\mathbf{X}')}{w(\mathbf{X})}\right]. \tag{2}$$

The probability density in *statistical physics* given by Gibbs in the canonical ensemble is [19]:

$$w(\mathbf{X}) = \text{const} \cdot \exp\left(-\frac{U(\mathbf{X})}{k_{\text{B}} T}\right), \tag{3}$$

where k_{B} is the Boltzmann constant, T is the temperature, and U is the potential energy of the system. The meaning of variables x_i is defined by the system under consideration (e.g., for simple fluids, these variables are particle locations, while they are spin signs at gridpoints in the Ising model).

The transition between states in the conventional Monte Carlo process is made, in accordance with Eq. (2), by *the random change of one variable* x_i *at a time*. Therefore, the conventional Monte Carlo simulation is a local process, with the result that the main trouble of this process is its slowness. A slowing-down is inherent not only in the conventional Monte Carlo algorithm, it is a common problem for all *local* processes (e.g., Gauss–Seidel relaxation for discretized partial differential equations). The solution to this problem lies in introducing system changes of a more collective nature. In the case of partial differential equations, the fast convergence of solutions had been attained by multigrid algorithms [20]. These algorithms are looking for the solution representation on a sequence of lattices with increasingly larger meshsizes (coarser scales), combining the local processing on each scale with various interscale (interlattice) interactions.

A similar technique can be applied to the simulation of liquids. The space is discretizied, and the sets of coarse-level variables are defined at gridpoints of a sequence of lattices. The main idea of the multilevel approach is to equilibrate, on each level, only the modes with short (comparable with the level's meshsize) wave lengths. Long-wave modes with slow convergence at a given level are equilibrated at coarser levels, where their wave lengths are comparable with the meshsize. As a result, the multilevel process leads to the fast equilibration of all modes.

In order to realize the multilevel Monte Carlo algorithm, it is necessary to introduce the set of coarse-level variables and the probability density of the state defined by this set.

There are many possible ways to choose the set of coarse variables. A general criterion for the quality of this set is the speed of equilibration of a *compatible Monte Carlo* (CMC). By this, we mean a Monte Carlo process on the fine level, which is restricted to the subset of fine-level configurations compatible with a *fixed* coarse-level configuration. For example, if each coarse variable is defined as a certain local spatial average of several fine-level variables, the CMC should be confined to steps that keep all these local spatial averages invariant (by, e.g., changing a pair of fine-level variables at a time, keeping their sum unaltered). A *fast* CMC equilibration implies that, up to local processing, all equilibrium configurations are fully determined by their coarse-level representations (their local spatial averages).

In the framework of the multilevel Monte Carlo algorithm, only a *local* process is performed at each level, being defined in terms of the corresponding variables. For changing the variable with the number i, say, one can see from Eq. (2) that it is enough to use, instead of the Gibbs function defined by (3), the *conditional* probability $P(x_i \mid \mathbf{R_i})$, which defines the probability of the given value for the variable x_i, when the values of all other variables defined by the set $\mathbf{R_i} = \{x_1, ..., x_{i-1}, x_{i+1}, ..., x_N\}$ are fixed.

For example, in the case of simple fluids, on the finest (particle) level, the definition of conditional

probability follows from Eq. (2) and Eq. (3):

$$P(\mathbf{r}_i \mid \mathbf{R_i}) = \text{const} \cdot \exp\left(-\frac{u_i(\mathbf{R_i})}{k_\text{B}T}\right), \tag{4}$$

where $\mathbf{r}_i$ is the location of the i-th particle and

$$u_i(\mathbf{R_i}) = \sum_{j,\,(j\neq i)} \phi(\mid \mathbf{r}_i - \mathbf{r}_j \mid). \tag{5}$$

Here, $\phi(\mid \mathbf{r}_i - \mathbf{r}_j \mid)$ corresponds to the energy of a two-body interaction.

The *Conditional Probability* is defined exactly only on the finest level, where the motion of particles is continuous. In order to calculate the transition probabilities defined by Eq. (2) on coarse levels, the conditional probabilities *should be derived* for each coarse level. These conditional probabilities can be expressed in the form of a *Conditional Probability (CP) table*, which, in principle, tabulates numerically the probability distribution of any coarse-level variable, given the values of all others. Of course, not *all* other variables should be taken into account in practice: only a certain small neighborhood counts, due to the *near locality* property of the conditional probability. This property results from the fast CMC equilibration: see the discussion of near locality in [21]. The CP tables for any coarse level k are calculated by gathering the appropriate statistics during the Monte Carlo simulation *at the next finer level* $k-1$. Because of the near-locality property, no *global* equilibration is needed; the local equilibration is enough to provide the correct CP values.

Due to the property of near locality, on coarse levels with large meshsize, the states of neighbor gridpoints can sometimes be considered to be independent of their environment. In this case, an analytical approximation for a *Conditional Probabilities (CP) function* can be developed. Examples of CP functions will be considered in the next sections.

2. Perfect Gas Under Gravity

In order to introduce coarse-level variables, the simulation domain is divided into M disjoint parts (e.g., cubes) V_i^1 of equal volume with linear size h_1, $1 \leq i \leq M$ (each V_i^1, being associated with a gridpoint i of the first coarse-level lattice). Configurations of the *finest (particle)* level are mapped to the first coarse level by the operation of *coarsening*; this operation

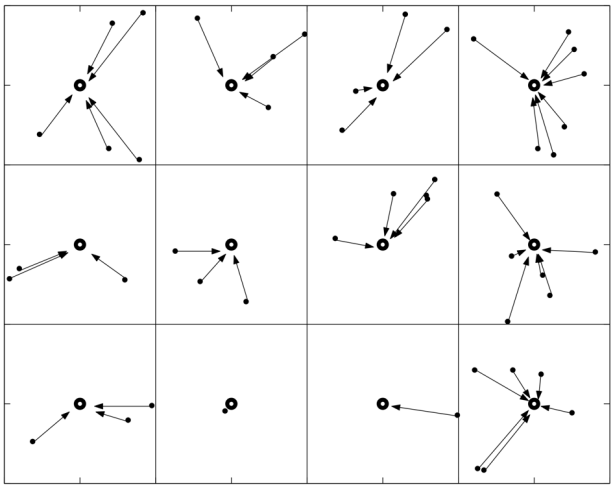

Fig. 1. Coarsening from the finest level to the first coarse level, ∘ denotes a gridpoint

creates the coarse-level variable set. For example, at any instant, the corresponding coarse-level variables can be defined in terms of the particle number:

$$n_i^1 = \text{ Number of particles in } V_i^1 \tag{6}$$

with $\sum_{i=1}^{M} n_i^1 = N$, where N is the total number of particles in the simulation domain.

The set $\{n_i^1\}$ defines the current configuration on the first coarse-level: instead of particle locations, the occupation numbers at gridpoints are used (see Fig. 1).

The extension of the coarsening operation given by Eq. (6) to coarser levels leads to the following definition of the coarse-variable at the level k:

$$n_j^k = \sum_{V_i^{k-1} \subset V_j^k} n_i^{k-1},\ k > 1 \tag{7}$$

for each volume element V_j^k of level k, assuming it to be a union of volume elements of the level $k-1$. The coarsening can be repeated to the coarsest level, whose choice depends on the scale of the phenomena one wants to compute.

In the case of perfect gas, all coarse-level variables defined by Eq. (6) and Eq. (7) are essentially statistically independent. This means that the neighboring coarse-level variables in Fig. 2 can be treated independently of all other variables. Under the assumption that the sum:

$$N_i = n_i + n_{i+1} \tag{8}$$

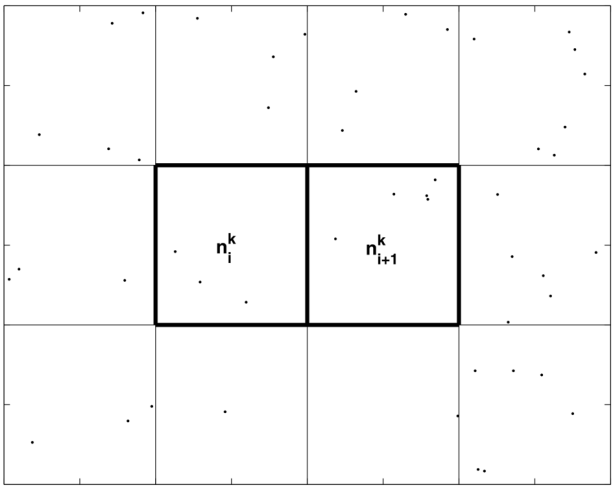

Fig. 2. Neighboring coarse-level variables

is fixed, the probability that the value of the coarse-level variable at gridpoint i is n_i follows from the usual consideration of the distribution of molecules of a perfect gas between two subdomains [22]:

$$P(n_i \mid N_i) = \frac{N_i!}{n_i! n_{i+1}!} p_i^{n_i} p_{i+1}^{n_{i+1}}, \tag{9}$$

where p_i is the probability that *any given particle* is in the subdomain i, i.e. is ascribed to the gridpoint i (obviously, $p_i + p_{i+1} = 1$). The probability p_i is a one-particle property; in the uniform gas, $p_i = p_{i+1} = 0.5$.

In a uniform gravitational field of acceleration g, each particle, which is placed at distance x from a reference point, has the energy

$$U(x) = mgx, \tag{10}$$

where m is the mass of a particle.

For two horizontally neighboring gridpoints (see Fig. 2) on a coarse level with meshsize h, in accordance with the Gibbs distribution given by Eq. (3), we have

$$p_i = \frac{1}{1+q}, \quad p_{i+1} = \frac{q}{1+q}, \tag{11}$$

where

$$q = e^{-\frac{mg}{k_B T} h}. \tag{12}$$

The quantity

$$\alpha = k_B T / mg \tag{13}$$

is called the gravitational length.

The approximation given by Eq. (12) is a consequence of the discretization of the space and coincides with the gravitational part of the lattice gas free energy functional [23].

In order to define a state of the two neighboring gridpoints shown in Fig. 2, it is convenient to introduce, in addition to Eq. (8), the variable

$$\Delta_i = n_i - n_{i+1}. \tag{14}$$

Substituting Eq. (11) into Eq. (9) and taking Eq. (14) into account, we find the desired form for the CP function:

$$P(\Delta_i \mid N_i) = \mathbf{C} \cdot \frac{q^{-\frac{\Delta_i}{2}}}{(\frac{N_i+\Delta_i}{2})!(\frac{N_i-\Delta_i}{2})!}, \tag{15}$$

where the quantity

$$\mathbf{C} = N_i! \left(\frac{q^{1/2}}{1+q}\right)^{N_i} \tag{16}$$

is independent of the difference Δ_i and, therefore, is unimportant for the calculation of the transition probability given by Eq. (2).

One can use the Stirling formula in order to transform Eq. (15) to a form suitable for numerical calculations at large occupation numbers:

$$P(\Delta_i \mid N_i) = \text{const} \cdot e^{-0.5 N_i \psi(\delta_i)}, \tag{17}$$

where $\delta_i = \Delta_i / N_i$ and

$$\psi(\delta_i) = (1+\delta_i)\ln(1+\delta_i) + \\ + (1-\delta_i)\ln(1-\delta_i) + \ln(q)\delta_i. \tag{18}$$

The most probable state is defined by the condition $\psi'(\delta_i) = 0$, which leads to the following *deterministic* equation in finite differences:

$$\Delta_i = \text{th}\left(\frac{mg}{2k_B T} h\right) N_i. \tag{19}$$

The CP function in the form given by Eq. (17) can be treated as the *stochastic* equation.

In the limit $h \to 0$, the usual differential equation for the density profile of a perfect gas in the external gravitational field follows from Eq. (19):

$$\frac{d\rho(x)}{dx} = -\frac{mg}{k_B T} t\rho(x), \tag{20}$$

where $\rho(x)$ is the *local* particle number density.

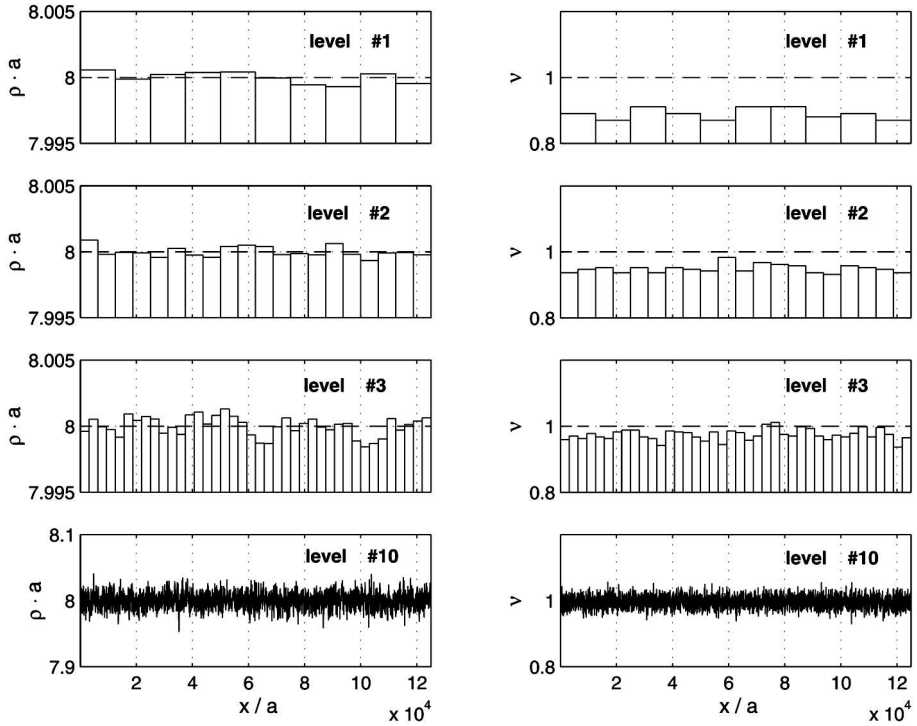

Fig. 3. Free perfect gas. The dashed line on the right-hand side corresponds to the bulk value of particle number fluctuation

In the case of a gas column of height L_x, the solution of this equation is:

$$\rho(x) = \overline{\rho}\frac{L_x}{\alpha(1-\exp(-L_x/\alpha))}\exp(-x/\alpha), \qquad (21)$$

where $\overline{\rho}$ is the mean value of the particle number density.

In a coarse-level Monte Carlo run, each trial move on the level k consists of the particle exchange between two neighboring gridpoints, i.e. $n_i^k \to n_i^{k'} = n_i^k + \Delta n$, $n_{i+1}^k \to n_{i+1}^{k'} = n_{i+1}^k - \Delta n$, where Δn is a random integer in the range $\mid \Delta n \mid < \Delta n_{\max}$, the acceptance rate of new configurations depends on the value of $\Delta n_{\max}$. The acceptance probability for this move is defined by Eq. (2). The CP function defined by Eq. (17) is used on all levels. This means that, in this case, the finest (particle) level is not included in the multilevel cycle. If the exchange of particles is done in the direction perpendicular to the x-axis, the gravitational term in the CP function is omitted.

The multilevel cycle begins from the coarsest level, and the runs are started from an initial uniform distribution of particles between gridpoints confined by the $x = 0$ and $x = L_x$ planes (in general, in the presence of gravity, it is enough to restrict the particle motion by the $x = 0$ plane). On the coarsest level, one can use a so large meshsize that the number of gridpoints will be relatively small; therefore, the equilibration is fast. To pass from a coarse level to the next finer level, one needs first to *interpolate*, i.e., to produce the fine level configurations represented by the current coarse level configuration. The interpolation is performed by CMC sweeps at the fine level (the meshsize at the next fine level is half the current one, and the number of gridpoints is larger by the factor 2^d, where d is the space dimension. Nevertheless, a small number of sweeps is enough, due to the fast CMC equilibration). The finest level is defined by the desired resolution.

After the equilibration on the fine level, the configuration *is coarsened* and returned to the coarse level, where simulations are resumed. The ensemble average properties of a system are estimated during these simulations at each level. When the coarsest level is attained, the multilevel cycle repeats, if necessary.

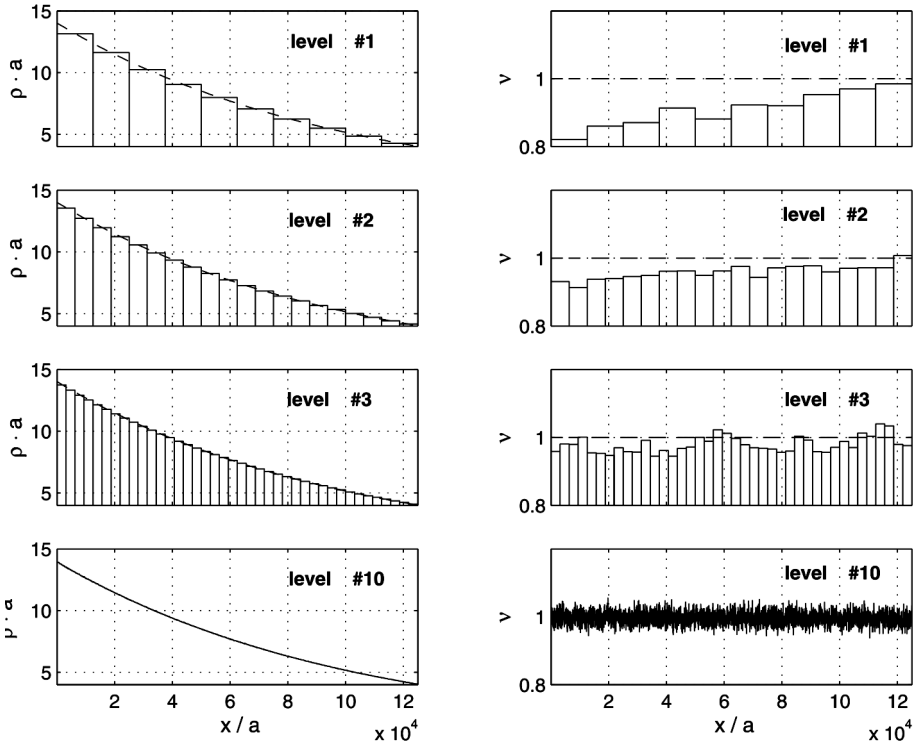

Fig. 4. Perfect gas under gravity. The dashed line on the left side corresponds to the exact density profile defined by Eq. (21). On the right side, the dashed line corresponds to the bulk value of the particle number fluctuation of a free gas

In order to test the multilevel algorithm, it was first applied to the simulation of a one-dimensional perfect gas in the absence of gravity. There is no relevant length scale in the free perfect gas. Therefore, an arbitrary length unit $\mathbf{a}$ is used. The simulation was performed for a system of 10^6 particles contained in a domain of size $L_x = 125000 \cdot \mathbf{a}$, which corresponds to the particle number density $\overline{\rho} \cdot \mathbf{a} = 8$. Ten gridpoints are introduced on the coarsest level numbered as level #1. The next fine level is numbered as level #2, *etc.*

The total number of levels in the simulation equals 10. The meshsize on the coarsest level is h_1, the meshsize on the i-th level is $h_i = h_1/2^i$. The multilevel run consists of 500 cycles, which corresponds to 30000 Monte Carlo sweeps on each level. Half of them is used for the calculation of average values of the particle number density and the fluctuation of the particle number:

$$\nu_i^k = \frac{\left\langle \left(n_i^k\right)^2 \right\rangle - \langle n_i^k \rangle^2}{\langle n_i^k \rangle} \tag{22}$$

at each gridpoint i of level k.

Results of the simulation are shown in Fig. 3. The mean value of the particle number density at each gridpoint slightly deviates from the average value over the whole simulation domain $\overline{\rho} \cdot \mathbf{a} = 8$. This disagreement decreases with increasing the amount of statistics. The same is true for the fluctuation of the particle number with one exception: the average value of the fluctuation on coarse levels is smaller than the bulk value of a perfect gas $\nu_{\text{bulk}} = 1$ [22]. This is caused by the finite-size effect; in the case of a perfect gas, the correction to the bulk value of the particle number fluctuation is given by [25]:

$$\nu_k = \nu_{\text{bulk}} \left(1 - \frac{h_k}{L_x}\right), \tag{23}$$

where h_k is the meshsize of level k. The result of the calculation of the average fluctuation at each level is shown in Fig. 5. One can see that the result is in agreement with Eq. (23).

Results for the example of a perfect gas under gravity in the case $h_1/\alpha = 0.125$ are shown in Fig. 4. The

simulation was performed under the same conditions as for the free perfect gas. The characteristic feature of the gas influenced by gravity is the nonuniform density profile. Therefore, the optimal choice of $\Delta n_{\max}$ has to be associated with the *local* particle number density. In the algorithm, the following simple relation between this quantity and the sum of the particle number at the two neighboring gridpoints under the trial move was used:

$$\Delta n_{\max} = n_c \sqrt{N_i}, \tag{24}$$

where n_c is a constant.

One can see from Fig. 4 that the density profile calculated by the Multilevel Monte Carlo method coincides with the exact result given by Eq. (21). The fluctuation of the particle number on finer levels is the same as in the free system. On the coarser levels, the fluctuation profile is nonuniform and increases in the low density tail. Nevertheless, the average fluctuations also conform to Eq. (23) (see Fig. 5).

3. Hard-Core Particle Fluids

In contrast to the case of a perfect gas, one can expect that the CP function for systems, which consist of finite-size particles, is reduced for the large values of particle number density. Therefore, the binomial distribution given by Eq. (3) has to be corrected. It was shown that the distribution of molecules between two subdomains in a lattice gas model is given by the hypergeometric distribution [26]. A further analysis has shown that the asymptotic representation of this distribution can be used successfully for the description of particle number fluctuations in continuous systems of hard disks and spheres [27]. Therefore, it is reasonable to use this approximation to develop the CP function for hard-sphere fluids.

In the framework of the lattice model, the distribution of particles between two subdomains is given by [26]:

$$P(n_i \mid N_i) = \binom{N_i}{n_i} \frac{\binom{M_i - N_i}{K_i - n_i}}{\binom{M_i}{K_i}}, \tag{25}$$

where M_i is the total number of lattice sites in the two subdomains (see Fig. 2), and K_i is the number of lattice cites in the subdomain i ($K_i + K_{i+1} = M_i$), $N_i = n_i + n_{i+1}$, being fixed.

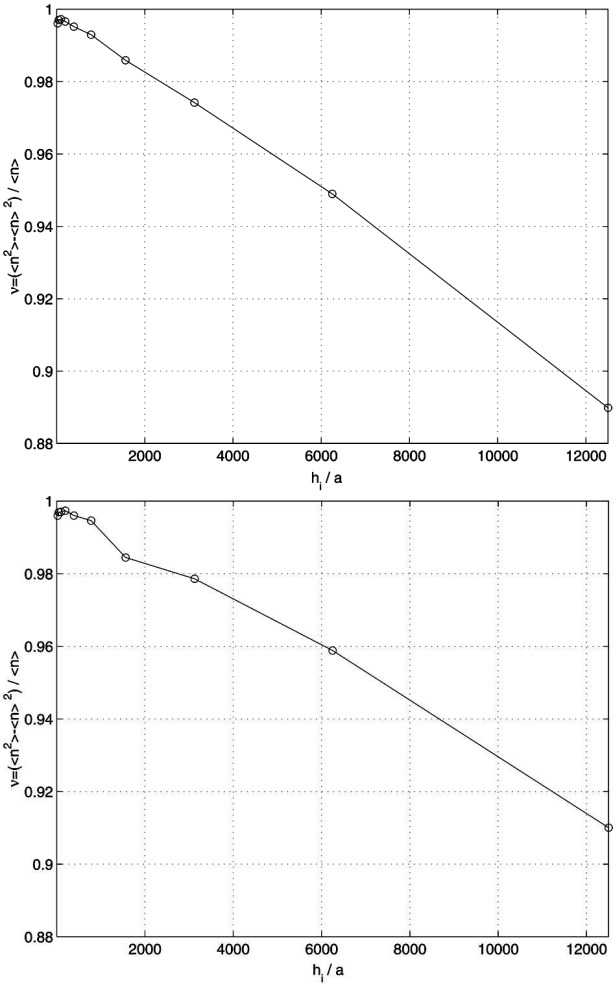

Fig. 5. Dependence of the particle number fluctuation in a subdomain on the meshsize for a free perfect gas (top panel) and a perfect gas under gravity (bottom panel)

The fluctuation of the particle number in the subdomain i follows from the dispersion for the distribution given by Eq. (25):

$$\nu_i = \frac{N_i}{n_i} \frac{K_i}{M_i} \frac{K_{i+1}}{M_i} \frac{1}{1 - 1/M_i} \left(1 - \frac{N_i}{M_i}\right). \tag{26}$$

If one subdomain, say i, is much smaller than the other one, i.e., under the condition $K_i \ll M_i$, $M_i \to \infty$, the fluctuation of the particle number can be associated with the isothermal compressibility κ [19]:

$$\nu_i = \rho k_{\mathrm{B}} T \kappa. \tag{27}$$

The interpretation of the quantity M_i for nonlattice models follows from Eq. (26) and Eq. (27):

$$M_i = \frac{N_i}{1-\chi}, \tag{28}$$

where $\chi = \rho k_{\mathrm{B}} T \kappa$ is the dimensionless isothermal compressibility.

Under the assumption that the relation defined by Eq. (28) is valid in continuous models (the interaction between particles results in the dependence of the isothermal compressibility on the particle number density), the CP function follows from Eq. (25) and Eq. (28), assuming $K_i = M_i/2$:

$$P(\Delta_i \mid N_i) = \mathbf{C} \cdot \frac{1}{(\frac{N_i+\Delta_i}{2})!(\frac{N_i-\Delta_i}{2})!} \times \\ \times \frac{1}{(\frac{N_i \frac{\chi}{1-\chi}+\Delta_i}{2})!(\frac{N_i \frac{\chi}{1-\chi}-\Delta_i}{2})!}. \tag{29}$$

The isothermal compressibility of a perfect gas is $\chi = 1$ [22]; in this case, Eq. (29) is reduced to Eq. (15) in the absence of an external field ($q = 1$). Therefore, the last term in Eq. (29) can be considered as a correction due to the finite particle size.

After applying the Stirling formula to Eq. (29), one obtains the CP function in the form of Eq. (17) with the following corrected definition of the function $\psi(\delta_i)$:

$$\psi(\delta_i) = (1+\delta_i)\ln(1+\delta_i) + (1-\delta_i)\ln(1-\delta_i) + \\ + (1+\frac{1-\chi}{\chi}\delta_i)\ln(1+\frac{1-\chi}{\chi}\delta_i) + \\ + (1-\frac{1\frac{\chi}{\chi}}{\chi}\delta_i)\ln(1-\frac{1\frac{\chi}{\chi}}{\chi}\delta_i) - \ln(q)\delta_i. \tag{30}$$

The *deterministic* equation in finite differences, which corresponds to Eq. (30), is defined by:

$$\Delta_i = \frac{1}{a}\frac{1-\sqrt{1-4(1-\chi)\chi a^2}}{2(1-\chi)}N_i, \tag{31}$$

where $a = \mathrm{th}(\frac{mg}{2k_{\mathrm{B}}T}h)$. If the gravitational length is much larger than the meshsize, Eq. (31) is reduced to the equation

$$\Delta_i = \frac{mg}{2k_{\mathrm{B}}T}h_i\chi N_i. \tag{32}$$

In the continuum limit $h_i \to 0$, one obtains the usual nonlinear differential equation for the density profile in a system of hard-core particles:

$$\frac{d\rho(x)}{dx} = -\frac{mg}{k_{\mathrm{B}}T}\chi\rho(x). \tag{33}$$

This equation coincides with the result of the density functional approach [14] and the consideration of the osmotic pressure in the sedimentation equilibrium of colloids [28, 29].

In order to use the CP function defined by Eq. (17) and Eq. (30) in the Multilevel Monte Carlo cycle, the isothermal compressibility should be derived. For that purpose, the following thermodynamical relation can be used [19]:

$$\frac{1}{\chi} = \left.\frac{\partial P/k_{\mathrm{B}}T}{\partial\rho}\right|_T, \tag{34}$$

where P is the pressure.

In the one-dimensional case, the exact equation of state is known [30]:

$$\frac{P}{k_{\mathrm{B}}T} = \frac{\rho}{1-\rho\sigma}, \tag{35}$$

where σ is the diameter of a particle. The exact isothermal compressibility for this system follows from Eq. (34) and Eq. (35):

$$\chi = (1-\rho\sigma)^2. \tag{36}$$

The differential equation for the density profile for a system of hard rods follows from Eq. (33) and Eq. (36):

$$\frac{d\rho(x)}{dx} = (1-\rho(x)\sigma)^2\rho(x). \tag{37}$$

Equation (37) can be integrated, and the density profile is defined by [14]

$$x/\alpha = \mathbf{C} - \frac{1}{1-\rho(x)\sigma} + \ln\frac{1-\rho(x)\sigma}{\rho(x)\sigma}, \tag{38}$$

where the coefficient $\mathbf{C}$ is defined by the wall contact value of local particle number density ρ_w :

$$\mathbf{C} = \frac{1}{1-\rho_w\sigma} - \ln\frac{1-\rho_w\sigma}{\rho_w\sigma}, \\ \rho_w\alpha = \frac{N_{\mathrm{tot}}}{1+N_{\mathrm{tot}}\sigma/\alpha}, \tag{39}$$

where N_{tot} is the total number of particles in the system.

The solution given by Eq. (38) is valid in semiinfinite space. Therefore, the comparison with the Monte

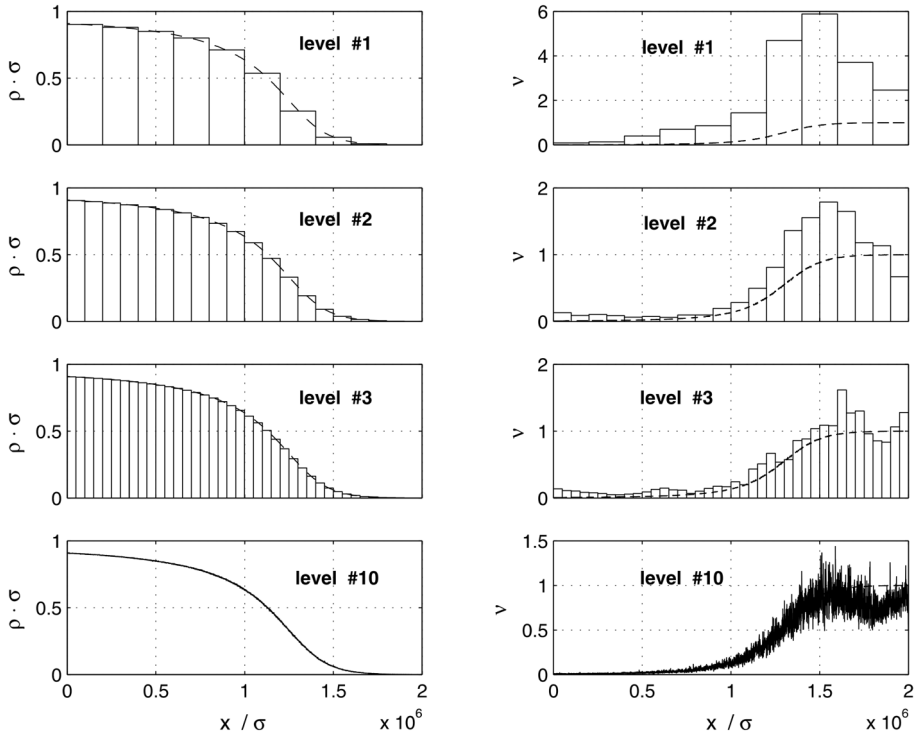

Fig. 6. Results of the multilevel Monte Carlo simulation for a system of hard rods. The dashed line on the left side corresponds to the analytical solution defined by Eq. (38). On the right side, the dashed line corresponds to the local estimation of the particle number fluctuation

Carlo result of a simulation in the confined space must be done carefully.

Results of the simulation for the mean value of particle number density $\overline{\rho}\sigma = 0.5$ and $h_1/\alpha = 2$ after five multilevel cycles (500 Monte Carlo sweeps at each level) are shown in Fig. 6. The density profile is in a very good agreement with the exact (for Eq. (37)) solution. The fluctuation of the particle number on the coarsest level considerably exceeds the expected value calculated by the particle number density at the subdomain in accordance with Eq. (36) (the local approximation). On finer levels, at least at the dense part of the density profile, this quantity coincides with the local estimation.

The exact equation of state for the system of hard disks is not available, but many empirical functions have been proposed. The simplest one follows from the scale particle theory [31]:

$$\frac{P_{\text{spt}}}{k_{\text{B}}T} = \frac{\rho}{(1-\eta)^2}, \tag{40}$$

where $\eta = \frac{\pi}{4}\rho\sigma^2$.

The expression for the isothermal compressibility is defined, in accordance with Eq. (34) and Eq. (40), by:

$$\chi_{\text{spt}}(\rho) = \frac{(1-\eta)^3}{1+\eta}. \tag{41}$$

The compressibility defined by Eq. (41) is zero at $\eta = 1$, which corresponds to the density $\rho\sigma^2 = 1.273$. However, the hard disk fluid crystallizes into the hexagonal structure at the density $\rho_c = 1.155$ ($\eta = 0.907$) [18]. Therefore, the isothermal compressibility for the hard disk fluid was defined by

$$\chi = \begin{cases} \chi_{\text{spt}}(\rho), & \rho \le \rho_c \\ 0, & \rho > \rho_c. \end{cases} \tag{42}$$

A six-level Multilevel Monte Carlo simulation was performed for the system of hard disks with the mean particle number density $\overline{\rho}\sigma^2 = 0.5$ and $h_1/\alpha = 7.07$. The system is confined in the x-direction; gravity acts along this axis. Periodic boundary conditions along the y-axis are assumed, the square simulation domain of the linear size $L = 141.42\sigma$ contains

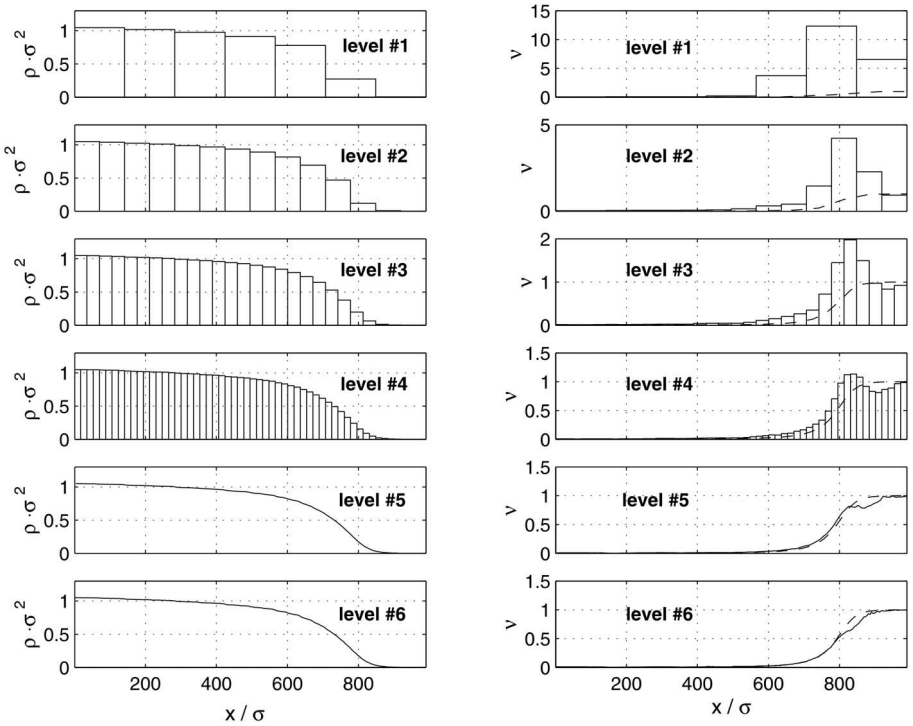

Fig. 7. Results of the multilevel Monte Carlo simulation for the system of hard disks. The dashed line corresponds to the local estimation of the particle number fluctuation. The density profile and the particle number fluctuation are averaged over the y-direction

10^6 particles. The equilibration of density profiles and fluctuations is attained after one multilevel cycle (200 Monte Carlo sweeps on each level), and the following modifications are small.

Results are shown in Fig. 7. A close-packing structure is formed at the bottom. Similar to the one-dimensional case, fluctuations at the dense part of the density profile coincide with the evaluation by the local approximation. This simulation result is in agreement with experimental data on the two-dimensional granular medium [32]. A clear disagreement is observed at the low density tail. The larger the scale, the larger the fluctuations.

4. Conclusions

The theoretical investigation of a number of problems in the physics of liquids, colloids, and fluidized granular materials is connected with the consideration of the external gravitational field. The present results show that the multilevel Monte Carlo method can be successfully applied for the investigation of a many-body system under gravity.

The conditional probability (CP) functions are developed, and it is shown that the correct *deterministic* differential equations can be derived from them in the continuum limit. At the same time, the CP function can be considered as the *stochastic* equation of state, which can be realized in multilevel Monte Carlo simulations. As a result, in addition to the average values of thermodynamic quantities (which can be obtained as the solution of the *deterministic* equation, if known), it is possible to estimate fluctuations.

It is known that fluctuations reflect the atomic structure of the matter [25]. In the CP function approach, the matter is considered via the isothermal compressibility, which is defined by the microscopic structure. For simple systems considered here, the isothermal compressibility can be derived from first principles. In the more widespread case, this quantity is unknown and can be obtained by simulation. In this case, the multilevel approach can again be ap-

plied, using CP *tables* [21], [24] instead of the CP function. The isothermal compressibility obtained in this way can be used in the CP function in order to simulate a system on the mesoscopic or macroscopic scale.

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А. Брандт, В. Ільїн, А. Скарбовійчук

ВЕЛИКОМАСШТАБНЕ МОДЕЛЮВАННЯ
РІДИН ПІД ДІЄЮ СИЛИ ТЯЖІННЯ

Р е з ю м е

Розроблено багатоторівневий метод Монте-Карло для моделювання рідин під дією сили тяжіння. В основі підходу умовні ймовірності станів, які можуть розглядатися як стохастичні рівняння для модельованої системи. Метод проілюстровано для прикладів ідеального газу і систем частинок з жорстким кором в одно- і двовимірюваннях, з використовуванням модельної функції умовної ймовірності.