Multilevel Approach in Statistical Physics of Liquids

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Abstract. A multilevel algorithm for molecular statistical investigation of liquids is described. The method is illustrated for a test case of the one-dimensional hard rods system, which is special in that it has analytic solutions.

1 Introduction

The modern theory of classical liquids is based on the statement that the macroscopic characteristics of a many-particle system can be obtained by averaging of microscopic configurations with the probability proportional to the Gibbs distribution function. Every microscopic configuration is defined by the current location of the particles and the main computational problem of statistical physics consists in the difficulty of averaging over this enormous space of possible configurations. In order to estimate the value of this average the Monte Carlo technique for the canonical ensemble was proposed [1].

However, the straightforward application of this technique is restricted to a small sub-volume of the system under consideration, because one can consider only a small number of particles in any numerical calculation. In order to minimize the surface effect on the bulk values which are to be calculated, artificial periodic boundary conditions are supposed [1] similar to the case of an infinite crystal [2]. This means that at the scale comparable with the periodicity cell size the fluctuations of the particle number are cut off. In order to avoid this difficulty several approaches have been suggested for the grand canonical ensemble [3],[4],[5]. The main trait of these algorithms is the generation of density fluctuation in the basic cell by adding and deleting particles in accordance with the value of the chemical potential.

The Monte Carlo simulations both in canonical and grand canonical ensembles are very local, moving, e.g., one particle at a time. This leads to very slow changes of large-scale features, such as averages and various types of clusters (regions of aligned dipoles, crystallized segments, etc.). The larger the scale the slower the change and longer is the Monte Carlo process required to produce new independent features. Since many independent features are needed for calculating accurate averages, and since very-large-scale features need to be sampled, especially in the vicinity of phase transitions, the computations often become extremely expensive, sometimes even losing ergodicity. In recent years, a number of novel Monte Carlo algorithms ensuring ergodicity were proposed [6], [7], [8]. In order to avoid the slowness of the ordinary Monte Carlo simulation, steps of more collective nature are used, overcoming the many-variable problems by multilevel algorithms [9],[10]. The multilevel algorithms construct a sequence of descriptions of the system under consideration at increasingly coarser levels and transfer information back and forth between the levels in order to obtain a selfconsistent result. The efficiency of multilevel methods in solving problems of statistical physics has been shown on examples with sufficiently simple systems [11]. It follows from these results that the effect of slowing down can be eliminated. Moreover, due to the possibility to simulate large volumes at coarse levels, the *volume factor* (the proportionality of the computational cost to the volume being simulated) can be suppressed as well. This means that the scale of treatment of a system is not restricted by the size of the basic cell. The elimination of both the slowing down and the volume factor allows one to investigate in the framework of the multilevel method long range phenomena such as phase transition. This possibility has been shown on examples of Gaussian models [11] and the Ising model [12].

The successful application of the multilevel methods to lattice systems excites interest in adapting them to more complicated cases. The present paper treats the general introduction of multilevel algorithms to the investigation of fluids. Numerical results of simulations for the one dimensional model of Tonks are presented. This model reproduces common properties of fluids and allows comparisons to an exact solution.

2 Outline of the Multilevel Approach

The motion of particles is continuous and in any configuration the particles have arbitrary locations. This standard description is the finest level of the multilevel algorithm. The Monte Carlo (MC) process produces configurations on this level in accordance with the Gibbs distribution for the canonical ensemble. The coarse levels all differ from the finest one in their nature, each coarse level is defined on a uniform *lattice*. A larger meshsize corresponds to a coarser level. The aim of coarsening is the creation of configurations represented by collective variables which describe collective motions of particles at different scales. Suitable variables should be chosen for each coarse level, and transition probabilities in terms of these variables should be derived.

The (scalar or vectorial) variable at each lattice point at each coarse level is defined as a *local spatial average* (an average or a sum over a certain neighborhood of the lattice point) of similar variables at the next finer level. Examples of such a variable are density (or mass), electrostatic charge, dipole moment, etc. The total value of each such variable per lattice cell is well defined for each configuration of particles and each lattice level.

A general criterion for the quality of the coarse-level set of variables is the speed of equilibration of any *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 whose local spatial averages coincide with a *fixed* coarse-level configuration. 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), which is the main desired property of coarsening.

The transition probabilities at each coarse level are expressed in the form of a *Conditional Probability (CP) table*, which in principle tabulates numerically the probability distribution of any one coarse-level variable Q_i given the values of all others, i.e., the probability distribution $P(Q_i \mid S_i)$, where $S_i = \{Q_1, Q_2, \ldots, Q_{i-1}, Q_{i+1}, Q_{i+2}, \ldots\}$. Of course, not *all* other variables should in practice be taken into account: only the immediate neighborhood of Q_i counts, due to the *near locality* property of the conditional probability. This is the property that for any subset $S_i' \subset S_i$, the difference $\mid P(Q_i \mid S_i) - P(Q_i \mid S_i') \mid$ decreases exponentially with the distance of the missing set $S_i - S_i'$ from Q_i. This property results directly from the fast CMC equilibration (cf.

discussion of near locality in [13]). Also, the conditional probability $P(Q_i \mid Q_{i_1}, Q_{i_2}, \ldots)$, where $i_1, i_2, \ldots$ are neighbors of i, need not be tabulated for all possible values of $Q_i, Q_{i_1}, Q_{i_2}, \ldots$. Only representative values should be tabulated; other values can be interpolated from the table. The table accuracy (in terms of the number of neighbors taken into account and the resolution in which each of them is tabulated) should in principle increase only around frequent values (cf. the branching system described in [13]).

The errors in such a description can be fully controlled by the choice of the neighborhood size, the table resolutions, the interpolation orders, and the amount of statistics gathered in setting up the tables.

The CP tables for any coarse level are calculated by gathering appropriate statistics (like those described in Sec. 3 below) during Monte Carlo simulations *at the next finer level*. Because of the near-locality property, no *global* equilibration is needed; local equilibration is enough to provide the correct CP values for any neighborhood for which enough cases have appeared in the simulation. Thus, the fine-level simulation can be done in a relatively small periodicity cell.

The idea is to simulate increasingly larger volumes at increasingly coarser levels.

However, since the fine-level canonical ensemble simulations use only a *small* periodicity cell, many types of neighborhoods that would be typical at some parts of a *large* volume (e.g., typical at parts with densities different than that used in the periodicity cell) will not show up or will be too rare to have sufficiently accurate statistics. Hence, simulations at some coarse level may run into a situation in which the CP table being used has flags indicating that values one wants to extract from it start to have poor accuracy. In such a situation, a temporary *local* return to finer levels should be made, to accumulate more statistics, relevant for the new local conditions.

To return 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, with correct relative probabilities. The interpolation is performed by CMC sweeps at the fine level; few sweeps are enough, due to the fast CMC equilibration. This fast equilibration also implies that the interpolation can be done just over a restricted *subdomain*, serving as a *window*: In the window *interior* good equilibrium is reached. Additional passes can then be made of *regular* (not compatible) MC, to accumulate in the interior of the window the desired additional CP statistics, while keeping the window boundary frozen (i.e., compatible). The window can then be coarsened (by the local spatial averaging) and returned to the coarse level, where simulations can now resume with the improved CP table.

Iterating back and forth between increasingly coarser levels and window processing at finer levels whenever missing CP statistics is encountered, one can quickly converge the required CP tables at all levels of the system, with only relatively small computational domains employed at each level. The size of those domains needs only be several times larger than the size of the neighborhoods being used (with a truncation error that then decreases exponentially with that size). However, somewhat larger domains are better, since they provide sampling of a richer set of neighborhoods (diminishing the need for returning later to accumulate more statistics), and since the total amount of work at each level depends anyway only on the desired amount of statistics, not on the size of the computational domain.

Simulating at all levels in terms of such cells and windows can effectively eliminate both the volume factor and the slowing down which plague usual (one-level) MC simulations. Provided of course that the *coarsening ratios* (the ratio between a coarse meshsize and the next-finer meshsize), as well as the average number of original particles per mash volume of the finest lattice, are all suitably low. The typical meshsize ratio is 2, typical number of particles per finest-lattice mesh is between 4 and 10. More aggressive coarsening ratios would require much longer simulations to accumulate accurate CP statistics.

The particle number density at the coarsest level is equal to the input value. Each finer-level window covers only part of the coarsest-level domain, so the particle number density may differ from the initial one. As a result of the multilevel process, the configurations produced at the coarsest level correspond to the canonical ensemble; at finer levels they approximate the grand canonical ensemble, as follows from its definition [15].

At sufficiently coarse levels, this entire algorithm effectively produces *macroscopic "equations"* for the simulated system, in the form of numerical CP tables. This can yield a macroscopic numerical description for the fluid even for those (most frequent) cases where the traditional derivation of closed-form differential equations is inapplicable.

Low temperature procedures. The multilevel algorithm can quickly get into equilibrium even at low temperatures by an *adaptive annealing* process. In this process the temperature is reduced step by step. At each step, upon reducing the temperature from a previous value T to a new one T', a first approximation to the CP tables of T' is obtain from those of T by raising each CP to the power T/T' (and renormalizing; actual renormalization is not necessary since only probability *quotients* are needed in using the CP table for MC simulations). Then, in just few multilevel cycles, the CP tables can easily be made more accurate, provided the quality of the set of coarse variables has not been deteriorated.

However, the type of coarse-level variables appropriate at low temperatures is generally different from that at high temperatures. At high temperatures the average density is an adequate coarse-level variable. At low temperatures, e.g., at the onset of piecewise crystallization, other coarse-level variables should be added, such as the average crystal direction, and/or the average density of holes, and/or the location of mass centers. Thus, in the annealing process one should monitor the quality of coarsening by occasionally checking the CMC equilibration speed. When this speed starts to deteriorate at some level, additional variables should be added at that level, with a corresponding extension of the CP table. Old variables may later be removable, as judged again by CMC equilibration tests.

Admittedly, all these multilevel procedures are rather elaborate, and require a gradual development of programs, insights and computational experience. We have started working on several rather simple models.

3 Algorithmic Details

The Monte Carlo method proposed in [1] is used to evaluate numerically the average $\overline{A}$ of any functional A, defined by:

$$\overline{A} = \int_{\Omega} A(\underline{X}) \cdot w(\underline{X}) \cdot d\underline{X} \approx \frac{1}{m} \sum_{i=1}^{m} A(\underline{X_i}) \, , \tag{1}$$

where $w(\underline{X})$ is the probability density of the state $\underline{X}$ in the configuration space Ω, and *the nodes* $\underline{X_i}$ are generated by a random walk in Ω that satisfies detailed balance. The simplest definition of the probability to walk from X_i to X_j in detailed balance is given by:

$$\omega(\underline{X_i} \rightarrow \underline{X_j}) = \min\left[1, \frac{w(\underline{X_j})}{w(\underline{X_i})}\right] , \tag{2}$$

provided the probability $P(X_j?|X_i)$ for choosing any state X_j as *the candidate* to replace a current state X_i is symmetric, i.e., $P(X_j?|X_i) = P(X_i?|X_j)$. The kind of state probability given by Gibbs is:

$$w(\underline{X}) = const \cdot \exp(-\frac{U(\vec{r_1}, \vec{r_2}, \ldots, \vec{r_N})}{k_B \cdot T}) \tag{3}$$

where k_B is the Boltzmann constant and T is the temperature. The potential energy U of the N-particle system is usually assumed to have the form:

$$U = \sum_{i<j} \phi(\mid \vec{r_i} - \vec{r_j} \mid) \tag{4}$$

where $\vec{r_i}$ is the location of the i-th particle ($i = 1, \ldots, N$), and $\phi(\mid \vec{r_i} - \vec{r_j} \mid)$ corresponds to the energy of a two-body interaction.

The transition between states on the finest level is made by the shift of one particle at a time. For shifting the particle with the number i, say, one can see from (2) that it is enough to use, instead of the Gibbs function (3) with the energy (4), the *conditional* probability defined by:

$$P(\vec{r_i} \mid \mathbf{R_i}) = const \cdot \exp(-\sum_{j,(j \neq i)} \phi(\mid \vec{r_i} - \vec{r_j} \mid)/k_B \cdot T) \tag{5}$$

The last relation gives us the probability to find the particle with the number i at the position $\vec{r_i}$ when the locations of all other particles, defined by the set $\mathbf{R_i} = \{\vec{r_1}, \ldots, \vec{r_{i-1}}, \vec{r_{i+1}}, \ldots, \vec{r_N}\}$, are fixed.

In order to introduce the variables of the first coarse level it is convenient to divide the basic cell into M parts (e.g., cubes) of equal volume V_j^1, $1 \leq j \leq M$. Each part is associated with a gridpoint j of the coarse-level lattice and the corresponding coarse-level variable is defined by:

$$n_j^1 = \quad Number\ of\ particles\ in\ V_j^1 \tag{6}$$

Note that such variables were used in the framework of a block density distribution technique which allows to extract information on the compressibility in the canonical ensemble [14]. The extension of this expression to coarser levels leads to the following definition of the coarse variables at the level k:

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

where $V_j^k = \cup V_i^{k-1}$ is a volume element of the coarser level.

At each coarse level the state of the system is described by variables (6), (7) defined at gridpoints. In terms of these variables conditional probabilities similar to (5) can be constructed in the following way. From a given sequence of configurations in equilibrium on the next finer level one can calculate the conditional probability table

$P(n_i \mid s_i^1,\ldots,s_i^l)$ which gives us the dependence of the probability to find n_i at the gridpoint i on l neighboring-point values defined by:

$$s_i^m = \sum_{j \in neighborhood\ of\ i} \alpha_{j-i}^m \cdot n_j, \ \ 1 \le m \le l \tag{8}$$

where α_{j-i}^m are preassigned, suitably chosen coefficients, $\alpha_0^m = 0$ for all m. For example a possible choice in one dimension is $l = 1$, $\alpha_i^1 = \begin{cases} 1, & i=\pm 1 \\ 0, & i \neq \pm 1 \end{cases}$.

On the coarse levels each trial move consists of particles exchange between two gridpoints, i.e. $n_i \rightarrow n_i' = n_i + \Delta n$, $n_t \rightarrow n_t' = n_t - \Delta n$. If i is not a neighbor of t (i.e., if $\alpha_{t-i}^m = \alpha_{i-t}^m = 0$ for all m), or if Δn is small, then, similarly to 2, the acceptance probability for this move is:

$$w(\underline{X}_{i,t} \rightarrow \underline{X}_{i',t'}) = \min\left[1, \frac{P(n_i' \mid s_i^1,\ldots,s_i^l)\cdot P(n_t' \mid s_t^1,\ldots,s_t^l)}{P(n_i \mid s_i^1,\ldots,s_i^l)\cdot P(n_t \mid s_t^1,\ldots,s_t^l)}\right] \tag{9}$$

With such a Monte Carlo process, equilibrium statistics is gathered in order to construct the conditional probability tables for variables defined by (7) on the *next* coarser grid. With these tables Monte Carlo simulations can now be made on that next level, and so on. The coarsening can be repeated till the coarsest level, whose choice depends on the given task.

In the coarse-to-fine interpolation, each coarse level particle number n_j^k should split its value between corresponding vertices of the finer lattice in accordance with (7). This is followed by a CMC simulation on the finer level, i.e., MC restricted by the condition that the values of the sums (7) remain unchanged. After performing a number of such CMC passes one obtains the fine-level equilibrium configuration which conserves the information from the coarser level. Similarly, in the interpolation to the finest level, the CMC particle simulation conserves (6).

4 Numerical Tests

In order to test the multilevel algorithm it was applied to the simulation of the one-dimensional hard rods system, defined by:

$$e^{-\frac{\phi(|\vec{r}_i-\vec{r}_j|)}{k_B T}} = \begin{cases} 1, & |\vec{r}_i-\vec{r}_j|>\sigma \\ 0, & |\vec{r}_i-\vec{r}_j|<\sigma \end{cases} \tag{10}$$

The main feature of many-body systems is the correlation of particle positions. In the perfect gas particles are uncorrelated. The solid state manifests a strong long-range order in position space. Liquids exhibit a short-range order, i.e., the correlation in particle positions vanishes with increasing the distance between them. The simplest model reproducing this structural property of liquids is the system of particles with the interaction defined by (10). The exact analytical solutions have been obtained in this case [18], and the equation of state, known as the Tonks equation, is:

$$\frac{P}{k_B T} \cdot \sigma = \frac{\eta}{1-\eta} \tag{11}$$

where σ is the diameter of a particle, P is the pressure and $\eta = \rho \cdot \sigma$ is the dimensionless density of the particle number.

First, *ordinary Monte Carlo simulations* were performed, both in the canonical and the grand canonical ensembles, using the same volume v^0 of the basic cell. It follows from (10) and (2) or (5) that the probability to move a particle is equal to 1 if particles after the displacement do not overlap. In the grand canonical ensemble the probability to add a particle at a random location to the basic cell when it already contains N particles is given [16] by:

$$\omega(\underline{X}_N \to \underline{X}_{N+1}) = \min\left[1, \frac{a \cdot v^0}{N+1}\right] \tag{12}$$

if the additional particle doesn't overlap with any of the existing N particles. The probability to remove a random particle is given by:

$$\omega(\underline{X}_N \to \underline{X}_{N-1}) = \min\left[1, \frac{N}{a \cdot v^0}\right] \tag{13}$$

where the value of the activity a is defined by the chemical potential μ ($a = e^{\frac{\mu}{k_B T}}/\Lambda^d$, d is the space dimension and Λ is the thermal wavelength [15]).

The activity in (12) and (13) in the case of the one-dimensional hard rods system is exactly known to be:

$$a = \frac{\eta}{1-\eta} \cdot \exp(\frac{\eta}{1-\eta}) \cdot \frac{1}{\sigma} \tag{14}$$

For the sake of measurements, the basic cell with the volume v^0 was divided into subdomains of equal volume $v^q = v^0/2^q$. For each value of $0 \le q \le q_{max}$ probabilities $p_q(n)$ of the particle number per volume v^q were tabulated, the width of bins being $\Delta n = 1$. This histograms allow to estimate simultaneously in a single simulation run the fluctuation ν_q of the particle number in subdomains of all sizes v^q into which the basic cell has been divided:

$$\nu_q = \frac{< n^2 >_q - < n >_q^2}{< n >_q} \tag{15}$$

where $< n >_q = \sum_n n \cdot p_q(n)$, $< n^2 >_q = \sum_n n^2 \cdot p_q(n)$.

In the thermodynamic limit (i.e., $v^0 \to \infty$, $N \to \infty$ at the condition $N/v^0 = \rho = const$) the fluctuation of the particle number does not depend on the volume v^q (if it is sufficiently large) and is related with the isothermal compressibility $\kappa = \left(-\frac{1}{V}\frac{\partial V}{\partial P}\right)_{T=const}$ [15]:

$$\frac{< n^2 > - < n >^2}{< n >} = \rho \cdot k_B T \cdot \kappa = (1-\eta)^2 \tag{16}$$

where the second equality follows from (11).

In the canonical ensemble the particle number N in the basic cell is constant, so $p_0(n) = \delta(n - N)$, $\delta(x)$ being the delta function. The value of the basic cell volume v^0 was chosen according to the average particle number density $v^0 = \frac{N}{\rho}$ (the value of N being kept constant in canonical ensemble simulations at different values of the particle number density ρ). In the grand canonical ensemble the same value of v^0 was used, the activity was calculated in accordance with (14), using the same value of $\eta = \rho \cdot \sigma$ as in the corresponding canonical ensemble run. For both ensembles, the measured distribution function $p_q(n)$ was used in order to estimate the right-hand side of (15).

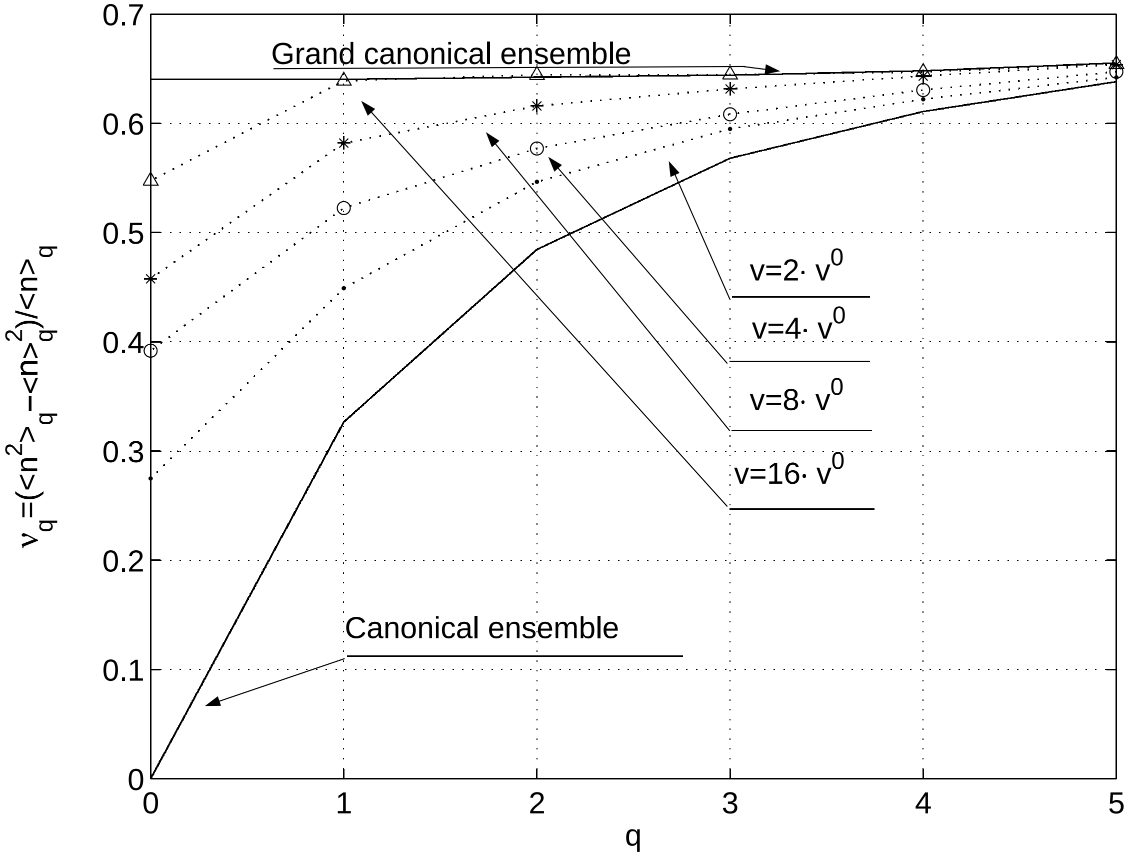

Figure 1: Detached lines show results of two-level calculations of the particle number fluctuation. The size of the coarse level basic cell changes in the interval $2 \cdot v^0 \leq v \leq 16 \cdot v^0$, where v^0 is the size of the finest level basic cell. Solid lines correspond to ordinary Monte Carlo simulations in canonical and grand canonical ensembles. The dimensionless particle number density is $\rho \cdot \sigma = 0.2$. The number of particles in v^0 is $N = 64$.

The results are shown by solid lines in Fig.1. Clearly, in the grand canonical ensemble the resulting ν_q exactly reproduce the value of the isothermal compressibility (16). In the canonical ensemble the isothermal compressibility is smaller and its value decreases with increasing of the volume of v^q (decreasing q).

Next, a *two-level* version of the multilevel algorithm was used. The coarse-level variable was introduced in accordance with (6), where V_j^1 was chosen to have the size $v^0/16$. In the special case of the one-dimensional fluid, the main contribution to the distribution of n_i at any lattice point i is expected to come from its nearest neighbors, therefore the conditional probability table $P(n_i \mid s_i)$ was used with only one variable s_i, defined by:

$$s_i = n_{i-1} + n_{i+1} \tag{17}$$

The algorithm starts with a Monte Carlo simulation at the fine level, in a periodicity domain of the volume v^0 containing $N = 64$ particles. Quantities of n_i and s_i are calculated at each lattice point i for each produced configuration, and from them the probability distributions $P(n_i \mid s_i)$ are accumulated, forming the CP table.

Then, coarse level Monte Carlo simulations are performed in accordance with (9), using this CP table and periodic boundary conditions. The size of the *coarse level* periodicity domain v was a constant that in different tests changed in the range $2 \cdot v^0 <$

$v < 16 \cdot v^0$. To still simulate the same average density, the total number of particles represented at the coarse level (i.e., $\sum n_i$) was kept at $N \cdot v/v^0$.

After that, a subdomain of the coarse level periodicity cell with volume v^0 is picked out randomly. The particle number contained in this subdomain generally *differs* now from N. The coarse level values of the variable n_i are interpolated to the fine (particle) level by CMC sweeps. Additional passes of the regular Monte Carlo algorithm are then made in that subdomain in order to update the CP table with additional statistics. Then the coarse Monte Carlo run resumes, with this improved table. Occasionally, the process returns from the coarse level to the fine level again in the same manner. In this way the fine level domain of volume v^0 contains *variable* particle number, similar to the case of the grand canonical ensemble, but each particle number is automaticaly produced with the correct probability, and large variations in the particle number can occur from one iteration to the next.

Results of the particle number fluctuation in subdomains of size v^q of the coarse level periodicity cell are shown also in Fig.1. One can see from this figure that the fluctuation of the particle number increases and tends to the exact value upon increasing the domain v where the coarse level Monte Carlo simulation is performed. This confirms that the choice of the CP table variable (17) is sufficiently good in the case under consideration.

Note of course that in actual *multi*level runs, an increasingly larger periodicity cells v are created on increasingly coarser levels, so the amount of work depends only weakly (logarithmically) on the size of v.

5 Discussion

The problem of the correct reproduction of the particle number fluctuation requires careful consideration. Simulations in the grand canonical ensemble suffer from the difficulty that a particle insertion into the system has at times a very poor MC acceptance rate, especially when applied to condensed phases. Different approaches are therefore employed for altering the particle number in the periodicity domain, and the results depend on the chosen approach [5]. For example, in order to avoid this difficulty the *parallel* grand canonical MC algorithm has been proposed [19]. This method uses a set of canonical ensemble simulations at different densities for the computation of the grand canonical ensemble averages. Transitions between systems with different particle numbers in the periodicity domain, equivalent to an addition or a deletion step, are accepted with average addition/deletion probabilities. In contrast to (12) and (13), these average probabilities are independent of the current particle locations in the basic cell. Fluctuations predicted in the framework of this method are smaller than the values predicted by thermodynamics [19]. A promising approach to grand canonical molecular dynamic simulations [20] treats the particle number in the basic cell as a continuous variable . However, simulation results, when compared to grand canonical MC data, show essential differences in the particle number fluctuation [21].

It follows from the present results that in the framework of the multilevel approach a suitable choice of coarsening allows to attain the macroscopic behaviour. The simple two-level example shows that if the size of the periodicity domain on the *coarse* levels is sufficiently large, the particle number fluctuation in subdomains of intermediate sizes tends to the exact value.

The multilevel algorithm is not concerned with the equilibrium between relative small subsystems in accordance with the value of a chemical potential. The equilibrium on fine levels (and in particular the frequency of the appearance of a given particle number in the basic cell) is defined by the canonical ensemble configurations on coarser levels. The accuracy of averages (including the particle number fluctuations) depends only on the CP tables adequacy, which is achieved by the correct selection of the variables set (8).

There is no phase transition in the hard core model. In order to study the influence of attractive forces on the gas and liquid state properties we are performing further investigations in this area for higher dimensional systems with a Lennard-Jones fluid.

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