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Multilevel Monte Carlo methods for studying large scale phenomena in fluids

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1. INTRODUCTION

The main computational problem of statistical physics consists in the difficulty of averaging over the 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].

The Monte Carlo simulations both in canonical and grand canonical ensembles are very local. 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 practical ergodicity.

An approach which allows to simultaneously overcome slowness and finite size effects of the conventional Monte Carlo method consists of a multilevel view of the system, realized by multilevel algorithms [2], [3]. The efficiency of multilevel methods in solving problems of statistical physics has been shown on examples with sufficiently simple systems [4].

The successful application of the multilevel methods to lattice systems excites interest in adapting them to more complicated cases.

2. Conventional Monte Carlo Method

The Monte Carlo method in the statistical theory of liquids 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 $\underline{X}$ to $\underline{X'}$ in detailed balance is given by :

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

provided that the probability $P(\underline{X'}?|\underline{X})$ for having chosen the state $\underline{X'}$ as *the candidate* to replace the current state X is symmetric, i.e., $P(\underline{X'}?|\underline{X}) = P(\underline{X}?|\underline{X'})$.

The transition between states is made by *the shift of one particle at a time* [1] by a small amount. 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 , the *conditional* probability defined by:

$$P(\vec{r_i} \mid \mathbf{R_i}) = const \cdot \exp(-u_i(\mathbf{R_i})/k_B T) \tag{3}$$

where $u_i(\mathbf{R_i})$ is the energy of the particle with the number 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.

3. Coarse variables

A possible way to introduce a coarse description of liquid consists in the discretization of space. The periodicity cell is divided into M disjoint subdomains (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*, which creates the coarse-level variable set. For example, for each particle configuration the corresponding coarse-level variables can be defined by coarsening the particle number:

$$n_i^1 = \text{ Number of particles in } V_i^1 \tag{4}$$

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

The extension of the coarsening operation (4) to coarser levels is defined by:

$$n_j^k = \sum_{V_i^{k-1} \subset V_j^k} n_i^{k-1}, \ k > 1 \tag{5}$$

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 till the coarsest level, whose choice depends on the scale of the phenomena one wants to compute.

A general criterion for the quality of coarse variables set is the speed of equilibration of *compatible Monte Carlo* (CMC) runs. By this we mean Monte Carlo processes on the fine level which are each restricted to the subset of fine-level configurations whose local spatial averages coincide with a *fixed* coarse-level configuration.

4. Coarse-Level Transition Probabilities

In order to conduct coarse-level simulations, *conditional probabilities* similar to (3) should be derived for each level. Such conditional probabilities are expressed in the form of a *Conditional Probability (CP) table*, which in principle tabulates numerically the probability distribution of any pair of neighboring coarse-level variables given the values of all others.

For example, in terms of variables (4), (5) defined at gridpoints a conditional probability tables $P_k(n_i^k, n_j^k \mid s_{ij}^{k1}, \ldots, s_{ij}^{kl})$ can be constructed from a given sequence of configurations in equilibrium on the next finer level $k-1$. These tables give us the dependence of the probability to find n_i^k and n_j^k particles at the two neighboring gridpoints i and j on l values in their neighborhood by:

$$s_{ij}^{km} = \sum_{q \in \, neighborhood \, of \, i \, and \, j} \alpha_q^m \cdot n_q^k, \quad 1 \le m \le l \tag{6}$$

where α_q^m are preassigned, suitably chosen coefficients, with $\alpha_i^m = \alpha_j^m = 0$ for all m.

For example, in one dimension $j = i+1$ and a possible choice is $l = 1$, $\alpha_{i-1}^1 = \alpha_{i+2}^1 = 1$, otherwise $\alpha_q^1 = 0$.

Such tables are all one need to conduct coarse-level simulations that conserve the total number of particles. Indeed in the coarse level Monte Carlo run, each trial move consists of particle exchange between two neighboring gridpoints, i.e. $n_i^k \rightarrow n_i^{k\prime} = n_i^k + \Delta n$, $n_j^k \rightarrow n_j^{k\prime} = n_j^k - \Delta n$. In accordance with (2), the acceptance probability for this move is:

$$\omega(\underline{X} \rightarrow \underline{X}') = \min\left[1, \frac{P_k(n_i^{k\prime}, n_j^{k\prime} \mid s_{ij}^{k1}, \ldots, s_{ij}^{kl})}{P_k(n_i^k, n_j^k \mid s_{ij}^{k1}, \ldots, s_{ij}^{kl})} \right] \tag{7}$$

The CP tables for any coarse level k are calculated by gathering appropriate statistics during Monte Carlo simulations *at the next finer level* $k-1$. Because of the near-locality property [2],[5], no *global* equilibration is needed.

5. DISCUSSION

The multilevel method was applied for a test case of one-dimensional fluids. A suitable quantity for comparing simulation results at different levels is the fluctuation ν_k of the particle number in the subdomain of size V^k. For the hard rods system the dependence of this quantity on the subdomain size coincides with the expression of the grand canonical ensemble [6], and five levels are enough in order to achieve the bulk value (exact result follows from the Tonk's equation). In the case of the Lennard-Jones fluid this dependence is shown in Fig.1. At high temperatures the properties of the Lennard-Jones fluid are similar to the hard rods system. At low temperatures the behavior of fluctuations drastically changes. The results obtained indicate that in contrast to the hard rods system the Lennard-Jones system loss homogeneity at low temperatures on fine scales.

The advantage of the multilevel Monte Carlo method consists in fast convergence of measured mean values due to the selfconsistent equilibration on different levels, each mode being well equilibrated and sampled on grids with meshsize comparable with the wave lengths. The computational work on each level is proportional to the number of gridpoints
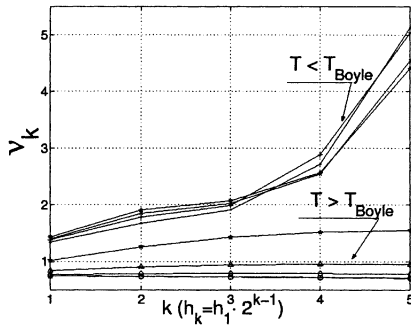
Figure 1. Particle number fluctuation at different levels (1D Lennard-Jones fluid, $h_1 = 2.5 \cdot \sigma$, $\rho \cdot \sigma = 0.2$. T_{Boyle} is the Boyle temperature.)

and is independent of the particle number associated with the gridpoint. It leads to the high speed of the method as compared with conventional algorithms.

The equilibrium on fine levels (and in particular the frequency of the appearance of a given particle number in the simulation domain) is determined by the canonical ensemble configurations on coarsest level. The particle number in fine level simulation domains is variable and its distribution agrees with the result of the grand canonical ensemble simulation [7]. The multilevel Monte Carlo method is not concerned with the equilibrium in accordance with the value of a chemical potential. It opens a new way for the development of a one-phase approach to the phase-transition problem [8].

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