

The optimum cut-off radius in Monte Carlo simulation of Yukawa potential point particles

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Abstract. In this paper, infinite systems of point particles with Yukawa potential and periodic boundary conditions are simulated using Monte Carlo technique in three dimensions. Because of the short range nature of the Yukawa potential, cut-off radius r_{cut} is considered in calculations (i.e, for each particle i , the effect of the other particles on it inside a sphere of radius r_{cut} is taken into account). The cut-off radius used in Monte Carlo simulation affects the physical behavior of the system being simulated. A sequence of r_{cut} values are used. When the change in the total potential energy becomes negligible, the optimum value of the cut-off radius is determined. This value is found to be independent of density and temperature in the NVT -ensemble case.

1. Introduction

Computer simulations of three-dimensional Yukawa fluids play a great role in many applications in Physics and Engineering. The short range nuclear forces produced from a meson interaction theory were proposed by Hideki Yukawa in 1935 [1]. According to this theory, each nucleon emits and reabsorbs pions in continuous behavior. The emitted pion may interact with new nucleon instead of returning to its parent nucleon. The resulting momentum, due to the shifting pions, is equivalent to the action of the nuclear forces. These forces are repulsive at very short ranges and attractive at large distances between nucleons. The static Yukawa potential (also called a screened Coulomb potential) is a spherically symmetric solution of the Klein-Gordon equation that takes the form [1]

$$V(r) = g \frac{e^{-\lambda r}}{r}, \quad (1)$$

where r is the distance between particles, λ and g are constants.

The Yukawa potential can be used to model the dynamical interactions between particles in plasmas and atomic physics [2]. The Monte Carlo simulation determined the phase diagram of a system consisting of hard core attractive Yukawa potential [3]. The fluid-solid phase transition was studied, and a transition curve was obtained for Yukawa systems near the one component plasma limit [4]. The location of the phase equilibrium and interfacial properties of two-dimensional Yukawa fluids were determined [5]. The linear and quadratic static density response functions of three-dimensional Yukawa liquid were computed by applying an external potential in molecular dynamics simulation [6]. The two-nucleon potential from the cut-off Yukawa theory was studied, and the two-nucleon interaction was



calculated up to the fourth order [7]. The melting line of the Yukawa system was located by determining the free energy of both fluid and solid phases by computer simulations [8]. In fact, many researches have been arising in the last and in the present centuries in the field of systems with Yukawa potential. The Yukawa potential is a short range one; hence, a cut-off radius of interaction can be used in simulations. The main goal of this research is obtaining the lowest cut-off radius that gives the total potential energy of the system. In order to achieve this purpose, Monte Carlo simulations are performed for the system at different values of temperature and density in an NVT -ensemble.

2. The cut-off radius

In the course of Monte Carlo simulation, the total potential energy is calculated before and after each Monte Carlo step. A straightforward simplification is truncating the interaction potential beyond a cut-off radius. The total Yukawa potential energy in this case is approximated by

$$U(r_{ij}) = \sum_{i < j} \bar{V}(r_{ij}), \quad (2)$$

where

$$\bar{V}(r) = \begin{cases} V(r), & r \leq r_{cut} \\ 0, & r > r_{cut} \end{cases}. \quad (3)$$

The accuracy of this approximation depends on the value of r_{cut} . In the case of Yukawa potential, r_{cut} can be typically chosen large enough such that the perturbation introduced into the simulation by the use of $\bar{V}(r)$ instead of $V(r)$ is negligible.

The potential truncation is generally possible if the particles effectively interact via short range pair potential. An important factor for the performance of Monte Carlo simulation code is its scalability with the number of particles in the system. Calculating all atomic interactions in the system during simulation is practically impossible. But, in systems with Yukawa potential, the inter atomic forces decreases rapidly by increasing the distance between particles; hence, considering the interactions within r_{cut} is reasonable. The optimal choice of r_{cut} is accomplished according to the fact that the difference between energy values approaches zero by increasing r_{cut} .

3. Numerical results

The simulation of Yukawa systems is performed by implementing periodic boundary conditions. The cubic box is replicated to form an infinite lattice. When a particle moves in the original box, its periodic images in other boxes move in the same way. In this work, N point-particles in the original box are simulated at fixed temperature T and fixed volume V . The number of particles used in calculations which is 125 is traditionally sufficient to get the desired results. The system under consideration is simulated in a cubic box using different values of r_{cut} , and the average value of the potential energy is calculated. For this purpose, the potential function (1) is reduced to

$$V(r_{ij}^*) = \frac{e^{-ar_{ij}^*}}{r_{ij}^*}, \quad (4)$$

where $a = g\lambda$, and $r_{ij}^* = \frac{r_{ij}}{g}$. Theoretically, using the reduced parameter $a = 1$ in simulations will give enough information about the optimum reduced value of the cut-off radius r_{cut}^* . The simulation is done at different values of temperature T^* and density ρ^* in the ranges $[0.5, 3]$ and $[0.25, 2]$, respectively. The convergence of Yukawa potential as a function of Monte Carlo sweep is tested. The reduced cut-off radius r_{cut}^* associated with large convergence speed and high accuracy is found. For example, figure 1 shows the average energy of the simulated system for $T^* = 2.5$ at different values of ρ^* and r_{cut}^* . The

main result that can be clearly noticed from figure 1 is that r_{cut}^* affects the average energy of the simulated system. By increasing the value of r_{cut}^* , the accuracy of the average potential energy becomes better until reaching a specific limit. Using cut-off radius greater than $r_{cut}^* = 3.5$ will give no significant change in the potential energy.

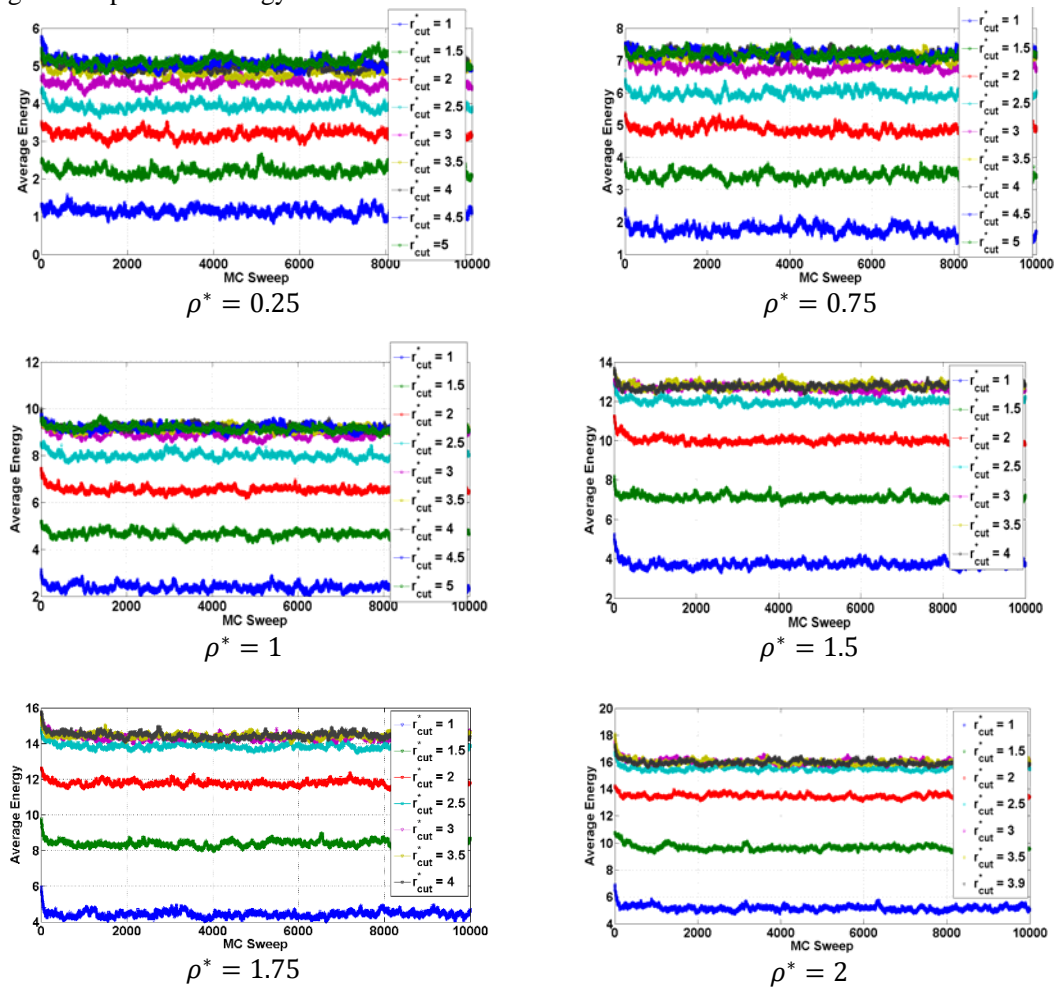


Figure 1. Average energy Versus Monte-Carlo sweeps for $T^* = 2.5$ at different values of ρ^* and r_{cut}^* .

The above procedure is repeated at many different values of ρ^* and T^* . In all cases, no remarkable change in the average potential energy happens at values of r_{cut}^* above 3.5. In addition, the fitting tool in MATLAB is used in order to obtain an equation that approximates the average energy in terms of density and Yukawa potential. The determination coefficient obtained is 0.9893. This approximation is formulated by

$$E(\rho^*, V) = 3.689 + 4.367\rho^* - 24.83V + 1.026(\rho^*)^2 - 11.58\rho^*V + 48.07V^2 \quad (5)$$

At $T^* = 0.5$ and $T^* = 1.5$, figure 2 shows the value of the reduced average energy difference $E_{r_{cut}^*}^i = U_{r_{cut}^*}^i - U_{r_{cut}^*}^{i-1}$, ($r_{cut}^* > r_{cut}^{i-1}$). The behavior shows that by increasing the cut-off radius, the difference in the total potential energy using any two successive values of r_{cut}^* approaches zero. In both cases, $r_{cut}^* = 3.5$ gives very accurate average energy.

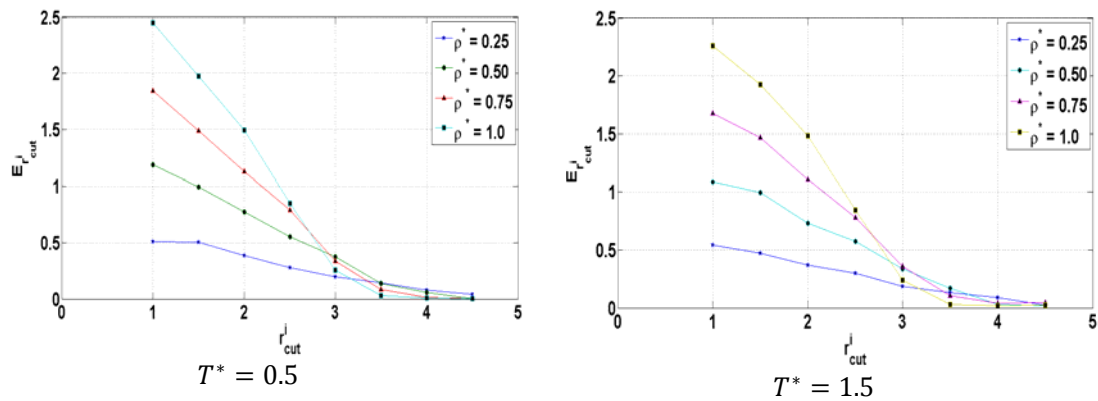


Figure 2. Energy difference at successive values of r_{cut}^* for $T^* = 0.5$ and 1.5 at different values of ρ^* .

4. Conclusions

One of the main goals of statistical physics is understanding the structure of liquids and gases from given inter particle interaction potentials. Major obstacles in this field are the limited range and the finite accuracy in measuring any observation. The Monte Carlo program used involves the calculation of the potential energy of a particular configuration. In principle, calculating the potential at any particle must include interactions of infinite number of terms which is not applicable in practice. Hence, in the course of simulation, an approximation using cut-off radius is used. The convergence of Monte Carlo simulation of N -particle system to the equilibrium state of Yukawa potential energy is affected by the cut-off radius. Increasing this radius increases the accuracy but causes a very slow convergence. The results of simulation at different values of temperature and density show that the reduced cut-off radius greater than 3.5 will not improve the accuracy. At all choices of temperature and density, the value 3.5 of the cut-off radius is optimum and using it in simulation makes it remarkably efficient.

Acknowledgments

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