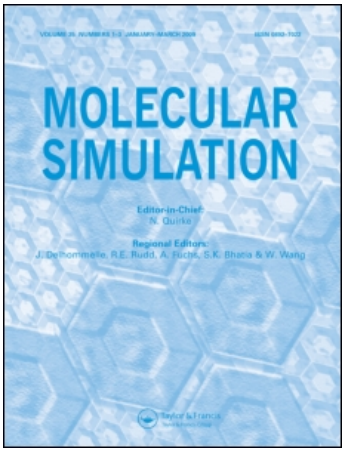

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"CHECKER BOARD" PERIODIC BOUNDARY CONDITIONS IN MOLECULAR DYNAMICS CODES

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Checker board periodic boundary conditions for molecular simulation are proposed. They represent a simple geometric transformation of the well known *periodic boundary conditions* formulae for variety of periodic and regular computational boxes (e.g. the truncated octahedron, rhombic dodecahedron, hexagonal prism, etc.) into a shifted parallelepiped periodic grid. As a result, the choice of an optional computational box shape is equivalent to the proper choice of the basic parallelepiped sides lengths.

The *checker board* periodic boundary conditions have been applied in a molecular dynamics (MD) code based on the link-cell method (using Lennard-Jones interactions). Simulation efficiency is approximately the same as for the *classical cubic* periodic boundary transformations.

KEY WORDS: Molecular dynamics, periodic boundary conditions, Lennard-Jones potentials, link-cell method, computational algorithms.

INTRODUCTION

Periodic Boundary Conditions (PBC) permit one to simulate bulk phase behaviour using limited number of N particles. The system of unlimited number of interacting particles is simulated by a limited number of interacting lattices where each of them is represented by a particle and its replicas. Drawbacks of the PBC approximation are evident [1], especially for simulation of some processes, e.g. for microscale hydrodynamics and phase transitions. When the distance between a particle and its nearest image, l_{NI}, is too small, long wavelength phenomena are neglected, and less valuable results are expected. Because l_{NI} scales as $N^{1/d}$ where d is the space dimension, double l_{NI} requires, for $d = 3$, eight times more particles, with considerable loss of simulation efficiency, since MD execution time scales as N^{ε}. (ε depends on algorithm order.)

For a given sample size, N, the distance l_{NI} is determined by the shape of the computational box. Usually the *cubic* box is used for the sake of simple "nearest images" determination. However, for the *Rhombic Dodecahedron* (RD) for example, l_{NI} is $\sim 12\%$ greater than for the simple cube. In order to get the similar l_{NI} as with RD simulation using the *cubic* box, approximately 40% more particles is needed. Moreover, RD simulates better isotrophic phase than the cube (see [1] and [2]). Adams [2] and Smith [3] have discussed four box shapes which could be alternatives to the periodic cube. They conclude that complicated transformation formulae appear to be the greatest disadvantage of the *non-cubic* computational boxes. This feature significantly reduces or even outweighs their advantages. Only one of the "exotic shapes", namely *Truncated Octahedron* (TO), seems to be attractive but its formulae are very difficult to vectorize. Moreover, the "exotic shapes" cannot be adopted for the

link-cell algorithm [5] for forces computation although the *link-cell* method is widely used due to its $o(N)$ complexity. When the box shape becomes more complicated (e.g. for sophisticated crystal lattice) the PBC transformations are prohibitively complex.

Recently Smith [4] has published a method for the minimum image convention in *non-cubic* MD cells. It is based on calculations performed in so-called fractional coordinates used for crystalline systems. Some additional matrix operations are needed in that case.

In the next sections the *cubic* PBC and some *non-cubic* alternatives are discussed. The idea of the checker board periodic conditions is presented. Timings of simple liquid MD simulations are shown and discussed.

CLASSICAL PERIODIC BOUNDARY CONDITIONS

Let the particles coordinates fulfil

$$\begin{aligned} x_i &\in (-L_X, L_X) \\ y_i &\in (-L_Y, L_Y) \\ z_i &\in (-1, 1) \end{aligned} \tag{1}$$

and $i = 1, \ldots, N$. The PBC transformations for the cuboidal box are as follows:

$$\begin{aligned} ix &= \mathrm{INT}(rx/L_X) \\ iy &= \mathrm{INT}(ry/L_Y) \\ iz &= \mathrm{INT}(rz) \\ rx &= rx - 2 * L_X * ix \\ ry &= ry - 2 * L_Y * iy \\ rz &= rz - 2 * iz \end{aligned} \tag{2}$$

where

$$\forall \alpha \in \{x, y, z\} \tag{3}$$

and

$$r\alpha = \begin{cases} \alpha_i & \text{for particle position calculations} \\ \alpha_{ij} = (\alpha_i - \alpha_j) & \text{for "nearest images" determination} \end{cases} \tag{4}$$

In the second case of Equation (4) j represents the neighbour particle to the i-th one. Additionally, the following condition must be performed

$$R_{CUT} \leqslant \min[\{L_X, L_Y, 1\}], \tag{5}$$

where

$$\min[\{L_X, L_Y, 1\}] = \frac{1}{2} l_{NI}. \tag{6}$$

R_{CUT} is the potential cutoff.

For other kinds of the computational box the formulae are more complex. They can be expressed as follows [3]

● for the RD box

$$
\begin{aligned}
ix &= \mathrm{INT}(rx/A)\\
iy &= \mathrm{INT}(ry/A)\\
iz &= \mathrm{INT}(rz/(\sqrt{2} * A))\\
rx &= rx - 2 * A * ix\\
ry &= ry - 2 * A * iy\\
rz &= rz - \sqrt{8} * A * iz \qquad (7)\\
&\textit{if}\ (\mathrm{ABS}(rx) + \mathrm{ABS}(ry) + \sqrt{2} * \mathrm{ABS}(rz)\ .\mathrm{LT.}\ 2 * A)\ \textit{then}\\
&\quad rx = rx - \mathrm{SIGN}(A, rx)\\
&\quad ry = ry - \mathrm{SIGN}(A, ry)\\
&\quad rz = rz - \mathrm{SIGN}(\sqrt{2} * A, rz)\\
&\textit{endif}
\end{aligned}
$$

where the longest diagonal of the RD face is equal to $2 * A$.

● for the TO box

$$
\begin{aligned}
ix &= \mathrm{INT}(rx/A)\\
iy &= \mathrm{INT}(ry/A)\\
iz &= \mathrm{INT}(rz/A)\\
rx &= rx - 2 * A * ix\\
ry &= ry - 2 * A * iy\\
rz &= rz - 2 * A * iz \qquad (8)\\
&\textit{if}\ (\mathrm{ABS}(rx) + \mathrm{ABS}(ry) + \mathrm{ABS}(rz)\ .\mathrm{LT.}\ 1.5 * A)\ \textit{then}\\
&\quad rx = rx - \mathrm{SIGN}(A, rx)\\
&\quad ry = ry - \mathrm{SIGN}(A, ry)\\
&\quad rz = rz - \mathrm{SIGN}(A, rz)\\
&\textit{endif}
\end{aligned}
$$

where the height of the TO box is equal to $2 * A$.

In order to summarize features of the boxes define

$$\eta = \text{(inscribed sphere volume)/(box volume)}, \qquad (9)$$

and

$$\lambda = \text{(circumscribed sphere volume)/(box volume)}. \qquad (10)$$

The main features of the RD, TO and *cubic* boxes are presented in Table 1 ([2]). SC reports the *Simple Cube*.

In addition, RD gives the maximum distance between a particle and its periodic

Table 1 Comparison of computational boxes

	lattice	η	λ
RD	fcc	$\pi\sqrt{2}/6$	$2\pi/3$
TO	bcc	$\pi\sqrt{3}/8$	$5\pi\sqrt{5}/24$
SC	–	0.52	2.72

image in comparison with other shapes, while TO box may fairly be described as the most "spherical" of all shapes.

Advantages of the RD and TO computational boxes in comparison with the *cubic* one are evident. However, the complicated forms of Equations (7–8), greater number of arithmetic operations, additional *if* statement and the standard functions – reduce them considerably. Moreover, vectorization of the code fragments (Eqs. (7–8)) is not efficient and programs which use them are slower than using the *simple cube* algorithm [2].

"CHECKER BOARD" PERIODIC BOUNDARY CONDITIONS

The *classical cubic* PBC and the *Checker board* Periodic Boundary Conditions (CPBC) are shown in Figures 1a and 1b respectively. For 2-D case the basic *Checker*

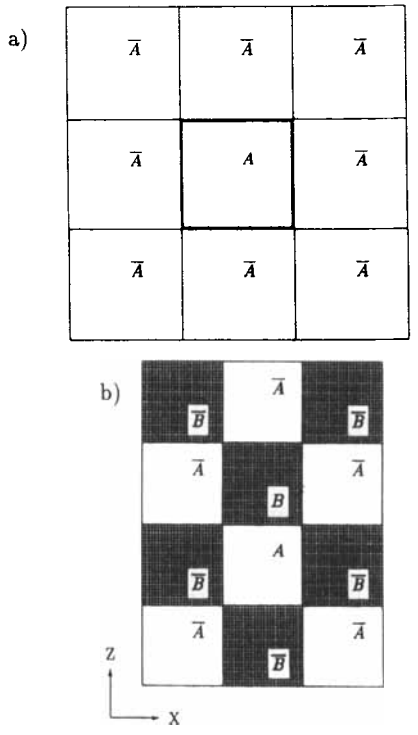

Figure 1 *Cubic* and *checker board* PBC box (2-D case).

Board computational box (CB), with sides lengths equal to $2L_X$ and $2L_Z$ respectively, consists of two similar rectangles, consists of two similar rectangles of the same size: *white* - *A* and *black* - *B*. Unlike to the periodic square, its replicas are shifted each other creating the checker board picture. The line connecting a particle (from *A* or *B*) and its nearest image (from $\bar{A}$ or $\bar{B}$ respectively) in Figure 1b, is parallel to diagonal of the *white* and *black* rectangles, while in Figure 1a the line connecting the particle and its image is parallel to the computational box side. For properly selected sides lengths of *white* and *black* rectangles, assuming that the (*A*–*B*) computational box area, *S*, is constant, a maximum of distance between a particle and its image can be obtained.

For *cubic* PBC – $l_{NI} = \sqrt{S}$. However, for CPBC and the basic box with side to side ratio $\kappa = L_Z/2L_X = 1/\sqrt{3}$, the distance between particles and their images from *A* and $\bar{A}$ (or from *B* and $\bar{B}$) is equal to

$$l_{NI} = a * \sqrt{S}, \tag{11}$$

where

$$a = \sqrt{2/\sqrt{3}} > 1. \tag{12}$$

Let S_C be area of the cicle $C(0,\frac{1}{2}l_{NI})$. The ratio, $\eta = S_C/S$, gives

$$\eta = \pi/(2\sqrt{3}), \tag{13}$$

which is approximately equal to 0.91. The effect is the same as for the *hexagonal* periodic box. The explanation of this fact is presented in Figure 2.

The CPBC turn out to be a result of the *hexagonal* grid transformation into the rectangular one. Empty rectangles in Figure 2 correspond to the *black* ones in Figure 1b and "dashed" - to the *white*, respectively. Moreover, the *rhombus* grid (see Figure 2b) is transformed into the same *checker board* grid as the *hexagonal* one. We can suppose that CPBC simulate a wide class of equivalent periodic structures.

For 3-D space CPBC give more profitable effects. The basic computational box consists of the *white* and the *black* parallelepipeds. The *black* one lies upon the *white* parallelepiped. Replicas of the computational box form black and white *checker board* system. Edges are common for the same "colors" only. (For 2-D case only vertices of the same "color" are common.)

Assume that:

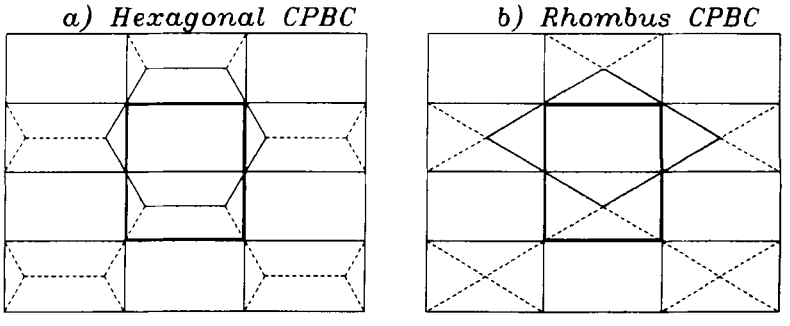

Figure 2 Equivalents of the *checker board* PBC box (2-D case).

- 3-D CPBC are considered,
- the particles coordinates perform conditions (1),
- the *white* and the *black* parallelepiped edges lengths are equal to: $2L_X$, $2L_Y$ and 1, respectively.

In such a case the distance between a particle and its nearest image is equal to:

$$l_{NI} = \sqrt{L_1^2 + L_2^2}, \tag{14}$$

where

$$\begin{aligned} L_1 &= \min\left[\{2L_X, 2L_Y, 1\}\right] \\ L_2 &= \min\left[\{2L_X, 2L_Y, 1\} - \{L_1\}\right] \end{aligned} \tag{15}$$

The transformation formulae can be written as follows

$$\begin{aligned} ix &= \mathrm{INT}(rx/L_X) \\ iy &= \mathrm{INT}(ry/L_Y) \\ iz &= \mathrm{INT}(rz + 2) \\ jj &= ix + iy \\ rz &= rz + B(iz, jj) \\ rx &= rx - 2 * L_X * ix \\ ry &= ry - 2 * L_Y * iy \end{aligned} \tag{16}$$

assuming that conditions (3–5) are valid. Auxiliary array, B, can be easily generated (see Figure 3). For 3-D case, it has a form presented in Table 2.

Table 3 contains L_X and L_Y values which should be substituted to Eq. (16) in order to obtain, by means of 3-D CPBC, simulation conditions equivalent to the classical

```
      SUBROUTINE BGENER(B)
      PARAMETER (IDIM = 2)
*****************************************
*        SPACE DIMENSION = IDIM + 1     *
*****************************************
      DIMENSION B(0:3, -IDIM:IDIM)
      DO 1 IZ = 0, 3
         B1 = -2 * INT (IZ-1.5)
         B2 = -2 * INT (IZ/2) + 1
         DO 10 JJ = -IDIM, IDIM
            IF (MOD (JJ, 2) .EQ. 0) THEN
               B(IZ, JJ) = B1
            ELSE
               B(IZ, JJ) = B2
            ENDIF
10       CONTINUE
1     CONTINUE
      RETURN
      END
```

Figure 3 Procedure for B generation.

Table 2 Array *B*

iz	*jj*				
	−2	−1	0	1	2
0	2	1	2	1	2
1	0	1	0	1	0
2	0	−1	0	−1	0
3	−2	−1	−2	−1	−2

Table 3 *Checker board* PBC parameters for different boxes

	L_X	L_Y	L_Z
RD	$\frac{1}{2}$	$\frac{1}{2}$	1
TO	$\frac{1}{2}$	$\frac{1}{\sqrt{8}}$	1
HP	1	$\frac{\sqrt{3}}{2}$	1
SC	$\frac{1}{2}$	$\frac{1}{\sqrt{2}}$	1

PBC for desired computational box shape (for 2-D case see Figure 2). HP stands for the *hexagonal prism*.

Obviously, CB consisting of two cubes (the first row in Table 3) does not refer only to the RD periodic grid but represents a wide class of various grids which are entirely equivalent (see Figures 2a and 2b). Changing L_X and L_Y we can choose optimal conditions for a computer experiment. For example, to get a maximum value of l_{NI} we have to use the formula represented by Equation (16), substituting L_X and L_Y by values given in the first row of Table 3.

In comparison with *non-cubic* PBC transformations given by Eqs. (7–8), the advantage of the transformation (16) is evident. For the case $L_X = L_Y = \frac{1}{2}$ in Eq. (16) (i.e. the RD box is used, see Table 3), the small overhead is needed only in comparison with the *simple cube* PBC represented by Equation (2) with $L_X = L_Y = 1$.

"CHECKER BOARD" PBC IN MD PROGRAM

Non-cubic PBC are extremely inconvenient for the *link-cell* method. Instead, CPBC can be used.

For test purposes CPBC have been applied in a MD code (written in C language [6], [7]) for simulation of monoatomic molecular mixtures which are modelled by site-site Lennard-Jones 12-6 interactions. The code is based on the *link-cell* algorithm. The timings presented below to the Ar/Kr mixture simulation for standard physical conditions ([6]), i.e. temperature is equal to 116 K and $R_{CUT} = 2.5\sigma_{Kr}$. (σ_{Kr} is the Lennard-Jones potential parameter for Kr.) The results have been obtained on the

Table 4 Execution time per timestep and particle (AT-386/20 MHz).

	τ, $10^{-3}s$/*timestep*/*particle*	
	checker board PBC	*classical cubic PBC*
RD	5.8	-
TO	6.0	-
HP	5.9	-
SC	5.9	5.8

AT-386 microcomputer (supported with i80386/387 microprocessor, 1MB RAM, 20 MHz), using MetaWare High C Compiler v1.4.

For the *link-cell* method the computational box is divided into sub-cells. Instead of the *nearest image* transformation (Equations (2) and (16)), in the *link-cell* algorithm auxiliary arrays can be used to identify boundary conditions:

$$\begin{aligned} rx_{ij} &= x_i - x_j + convx \\ ry_{ij} &= y_i - y_i + convy \\ rz_{ij} &= z_i - z_j + convz \end{aligned} \tag{17}$$

For *classical cubic* PBC

$$\begin{aligned} convx &= N\,convx\,(jcellx) \\ convy &= N\,convy\,(jcelly) \\ convz &= N\,convz\,(jcellz) \end{aligned} \tag{18}$$

while for CPBC

$$\begin{aligned} convx &= N\,convx\,(jcellx) \\ convy &= N\,convy\,(jcelly) \\ convz &= N\,convz\,(jcellx, jcelly, jcellz) \end{aligned} \tag{19}$$

In the above equations *jcellx*, *jcelly* and *jcellz* are neighbouring cells coordinates, see [8].

Because auxiliary arrays are initialized once only, the efficiencies of the MD codes which use *classical* PBC and CPBC should be similar. For the second case little overhead is observed (see Table 4) due to the *non-cubic* shape of the sub-cells and 3-dimensional *Nconvz* table. (The optimal efficiency for *link-cell* method is obtained if $R_{CUT} = l$, where l is the cubic sub-cell side length [8].)

CONCLUDING REMARKS

- The *checker board* PBC are more universal than the classical ones. By means of the computational box made of parallelepipeds, it is possible to simulate optional periodic grids (*truncated octahedron*, *rhombic dodecahedron*, its mutations, etc.), changing the size of the basic computational box only, without any changes in the general formulae.
- The *checker board* PBC transformations and *nearest images* determination are more efficient than those obtained earlier for the *non-cubic* PBC. The formulae

(16) are almost as efficient as for the simple periodic cube one, so that the net effect of the *non-cubic* PBC advantages (i.e. l_{NI} increase) is obtained. Using the *checker board* PBC with $L_X = L_Y = \frac{1}{2}$ for simulation of dynamics of N particles we get the same l_{NI} distance as for $\sqrt{2N}$ particles using *classical cubic* PBC. As a result, gain of simulation efficiency is observed.

- The *link-cell* method can easily be applied in the *checker board* PBC. As a result, large particle systems of various kinds of the computational box can be simulated due to high efficiency of the *link-cell* method.
- Some explanation on efficiency is needed if one choses to use the *checker board* computational box together with the *link-cell* technique. In such a case the computational box is divided into smaller sub-cells for which *linked-lists* are applied. The highest efficiency is obtained if the sub-cells are cubical, since the potential cutoff is properly inscribed into sub-cell structure. This requirement is fulfil for RD box due to its side lengths (see Table 2). For other boxes, e.g. TO or HP, the sub-cells are not cubical in general, which results in excessive calculations of distances between particles. (This drawback could be reduced by changing the number of particles to obtain better fitting of sub-cell size to the cutoff radius or using a more sophisticated algorithm, as for example the *sorted linked lists* method [9].) Instead, one gets the simple and efficient tool for simulation with unconventional boxes.
- The *checker board* PBC transformations can be easily extended to higher dimensions.
- Little effort is needed to apply *checker board* PBC in existing MD and MC programs.

The *checker board* PBC formulation seems to be a flexible and an efficient tool for molecular dynamics simulation and, maybe, for other kinds of computer simulation methods.

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