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Molecular Dynamics of Yukawa System using the Fast Multipole Method

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In order to perform the large-scale molecular dynamics simulation of the Yukawa system, a mathematical expression for molecular dynamics using the fast multipole method is described. The model simulations are also performed to test the performance of our implementation of the FMM.

1 Introduction

The statistical mechanics of the Yukawa system, the system of particles interacting via the Yukawa potential, has long been studied as models of simple but non trivial system [1]. The Yukawa potential smoothly interpolates the long-rang Coulomb and the short-range interactions by adjusting a single parameter, the screening length. As real systems where interactions are given by the Yukawa potential, we have classical and quantum plasmas, charge stabilized colloidal suspensions, and dusty plasmas [2, 3].

In order to perform molecular dynamics simulation of these systems, we need to calculate the forces acting on particles or the potentials where particles exist. For a system with relatively long screening length, we require computational complexity of $O(N^2)$ to calculate potential and forces, since the number of pairs of particles increases quadratically with respect to the number of particles N. This makes it impossible to perform a very large-scale simulation of these systems. The fast multipole method (FMM), developed by Greengard and Roklin [4, 5, 6], is a powerful algorithm to calculate long-range interaction. The FMM is able to reduce the computational complexity from $O(N^2)$ to $O(N)$. Furthermore, this method can be easily parallelized because of its hierarchical character.

In this paper, we describe mathematical expressions for molecular dynamics of Yukawa system using the FMM. The model simulations are performed to test the performance of our implementation of the FMM.

2 Fast Multipole Method

2.1 Basic idea

In this subsection, we first explain the basic idea of this method. In this method, the electrostatic potential Φ_{tot} at a given point is expressed as the sum of two parts,

$$\Phi_{tot} = \Phi_{near} + \Phi_{distant}, \tag{1}$$

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where Φ_{near} is the potential induced by nearby particles and obtained by directly calculating interactions between particles, whereas $\Phi_{distant}$ is the potential induced by distant particles and obtained by using the multipole and the Taylor expansions.

2.1.1 Multipole Expansion

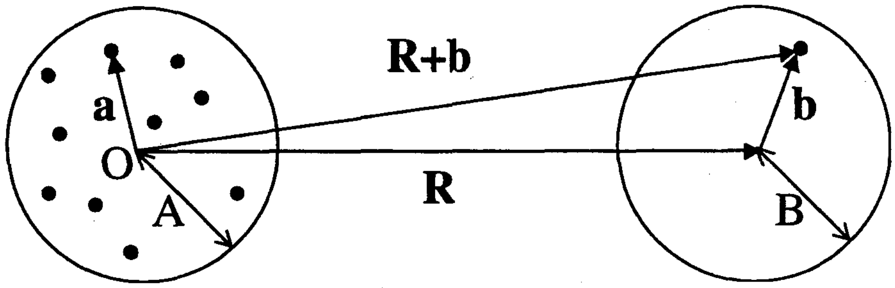


Figure 1: Multipole and Taylor expansion

We here consider the interactions between particles, each of which belongs to two distinct local regions that are well separated (Fig. 1). Suppose that M charged particles interacting via a potential $\phi(r)$ are located at positions $\{\mathbf{a}_i, i = 1, 2, \ldots, M\}$ within a sphere of radius A and have a charges of strength $\{q_i, i = 1, 2, \ldots, M\}$. Then the potential at a position $\mathbf{r}$ induced by the charges within the sphere of radius A is given by

$$\Phi(\mathbf{r}) = \sum_i q_i \phi(\mathbf{r} - \mathbf{a}_i). \tag{2}$$

If $|\mathbf{r}|$ is much larger than A, $\phi(\mathbf{r}-\mathbf{a})$ can be approximated by the first several terms of multipole expansion,

$$\begin{aligned}\phi(\mathbf{r}-\mathbf{a}) &= \phi(\mathbf{r}) - \sum_\alpha (\mathbf{a})_\alpha \phi_\alpha(\mathbf{r}) + \frac{1}{2!}\sum_{\alpha\beta}(\mathbf{a})_\alpha(\mathbf{a})_\beta\phi_{\alpha\beta}(\mathbf{r}) \\ &\quad - \frac{1}{3!}\sum_{\alpha\beta\gamma}(\mathbf{a})_\alpha(\mathbf{a})_\beta(\mathbf{a})_\gamma\phi_{\alpha\beta\gamma}(\mathbf{r}) + \frac{1}{4!}\sum_{\alpha\beta\gamma\delta}(\mathbf{a})_\alpha(\mathbf{a})_\beta(\mathbf{a})_\gamma(\mathbf{a})_\delta\phi_{\alpha\beta\gamma\delta}(\mathbf{r}) \\ &\quad - \frac{1}{5!}\sum_{\alpha\beta\gamma\delta\epsilon}(\mathbf{a})_\alpha(\mathbf{a})_\beta(\mathbf{a})_\gamma(\mathbf{a})_\delta(\mathbf{a})_\epsilon\phi_{\alpha\beta\gamma\delta\epsilon}(\mathbf{r}) \\ &\quad + \frac{1}{6!}\sum_{\alpha\beta\gamma\delta\epsilon\zeta}(\mathbf{a})_\alpha(\mathbf{a})_\beta(\mathbf{a})_\gamma(\mathbf{a})_\delta(\mathbf{a})_\epsilon(\mathbf{a})_\zeta\phi_{\alpha\beta\gamma\delta\epsilon\zeta}(\mathbf{r}).\end{aligned} \tag{3}$$

The potential is thus expressed as

$$\begin{aligned}\Phi(\mathbf{r}) &= M\phi(\mathbf{r}) - \sum_\alpha D_\alpha\phi_\alpha(\mathbf{r}) + \frac{1}{2!}\sum_{\alpha\beta}Q_{\alpha\beta}\phi_{\alpha\beta}(\mathbf{r}) \\ &\quad - \frac{1}{3!}\sum_{\alpha\beta\gamma}O_{\alpha\beta\gamma}\phi_{\alpha\beta\gamma}(\mathbf{r}) + \frac{1}{4!}\sum_{\alpha\beta\gamma\delta}H_{\alpha\beta\gamma\delta}\phi_{\alpha\beta\gamma\delta}(\mathbf{r}) \\ &\quad - \frac{1}{5!}\sum_{\alpha\beta\gamma\delta\epsilon}T_{\alpha\beta\gamma\delta}(\mathbf{a})_\epsilon\phi_{\alpha\beta\gamma\delta\epsilon}(\mathbf{r}) + \frac{1}{6!}\sum_{\alpha\beta\gamma\delta\epsilon\zeta}U_{\alpha\beta\gamma\delta\epsilon\zeta}\phi_{\alpha\beta\gamma\delta\epsilon\zeta}(\mathbf{r}),\end{aligned} \tag{4}$$

where $\{M, D_\alpha, \ldots\}$ are multipole moments defined as follows,

$$M = \sum_i q_i, \tag{5}$$

$$D_\alpha = \sum_i q_i(\mathbf{a}_i)_\alpha, \quad (6)$$

$$Q_{\alpha\beta} = \sum_i q_i(\mathbf{a}_i)_\alpha(\mathbf{a}_i)_\beta, \quad (7)$$

$$O_{\alpha\beta\gamma} = \sum_i q_i(\mathbf{a}_i)_\alpha(\mathbf{a}_i)_\beta(\mathbf{a}_i)_\gamma, \quad (8)$$

$$H_{\alpha\beta\gamma\delta} = \sum_i q_i(\mathbf{a}_i)_\alpha(\mathbf{a}_i)_\beta(\mathbf{a}_i)_\gamma(\mathbf{a}_i)_\delta, \quad (9)$$

$$T_{\alpha\beta\gamma\delta\epsilon} = \sum_i q_i(\mathbf{a}_i)_\alpha(\mathbf{a}_i)_\beta(\mathbf{a}_i)_\gamma(\mathbf{a}_i)_\delta(\mathbf{a}_i)_\epsilon, \quad (10)$$

$$U_{\alpha\beta\gamma\delta\epsilon\zeta} = \sum_i q_i(\mathbf{a}_i)_\alpha(\mathbf{a}_i)_\beta(\mathbf{a}_i)_\gamma(\mathbf{a}_i)_\delta(\mathbf{a}_i)_\epsilon(\mathbf{a}_i)_\zeta. \quad (11)$$

Here $\alpha, \beta, \ldots$ are any of x, y, z, $(\mathbf{a}_i)_\alpha$ is α-component of $\mathbf{a}_i$, and $\phi_{\alpha\beta\ldots}$ defines a derivative of ϕ with respect to $\alpha, \beta, \ldots$, respectively. Summation is over particles within the sphere of radius A. The number of multipole moments is $(p+1)(p+2)(p+3)/6$ when the potential is expanded up to the pth order. In this case $(p = 6)$, the number of multipole moments is 84.

2.1.2 Convert Multipole Expansion to Taylor Expansion

The potential at position $\mathbf{R} + \mathbf{b}$, which is multipole expanded above, can be Taylor expanded about $\mathbf{R}$ when $|\mathbf{R}| >> |\mathbf{b}|$,

$$\begin{aligned}
\Phi(\mathbf{R}+\mathbf{b}) = {} & M\Bigg\{\phi(\mathbf{R}) + \sum_\alpha \phi_\alpha(\mathbf{R})(\mathbf{b})_\alpha + \frac{1}{2!}\sum_{\alpha\beta}\phi_{\alpha\beta}(\mathbf{R})(\mathbf{b})_\alpha(\mathbf{b})_\beta \\
& + \frac{1}{3!}\sum_{\alpha\beta\gamma}\phi_{\alpha\beta\gamma}(\mathbf{R})(\mathbf{b})_\alpha(\mathbf{b})_\beta(\mathbf{b})_\gamma \\
& + \frac{1}{4!}\sum_{\alpha\beta\gamma\delta}\phi_{\alpha\beta\gamma\delta}(\mathbf{R})(\mathbf{b})_\alpha(\mathbf{b})_\beta(\mathbf{b})_\gamma(\mathbf{b})_\delta \\
& + \frac{1}{5!}\sum_{\alpha\beta\gamma\delta\epsilon}\phi_{\alpha\beta\gamma\delta\epsilon}(\mathbf{R})(\mathbf{b})_\alpha(\mathbf{b})_\beta(\mathbf{b})_\gamma(\mathbf{b})_\delta(\mathbf{b})_\epsilon \\
& + \frac{1}{6!}\sum_{\alpha\beta\gamma\delta\epsilon\zeta}\phi_{\alpha\beta\gamma\delta\epsilon\zeta}(\mathbf{R})(\mathbf{b})_\alpha(\mathbf{b})_\beta(\mathbf{b})_\gamma(\mathbf{b})_\delta(\mathbf{b})_\epsilon(\mathbf{b})_\zeta\Bigg\} \\
& - \sum_\alpha D_\alpha\Bigg\{\phi_\alpha(\mathbf{R}) + \sum_\beta\phi_{\alpha\beta}(\mathbf{R})(\mathbf{b})_\beta + \frac{1}{2!}\sum_{\beta\gamma}\phi_{\alpha\beta\gamma}(\mathbf{R})(\mathbf{b})_\beta(\mathbf{b})_\gamma \\
& + \frac{1}{3!}\sum_{\beta\gamma\delta}\phi_{\alpha\beta\gamma\delta}(\mathbf{R})(\mathbf{b})_\beta(\mathbf{b})_\gamma(\mathbf{b})_\delta \\
& + \frac{1}{4!}\sum_{\beta\gamma\delta\epsilon}\phi_{\alpha\beta\gamma\delta\epsilon}(\mathbf{R})(\mathbf{b})_\beta(\mathbf{b})_\gamma(\mathbf{b})_\delta(\mathbf{b})_\epsilon \\
& + \frac{1}{5!}\sum_{\beta\gamma\delta\epsilon\zeta}\phi_{\alpha\beta\gamma\delta\epsilon\zeta}(\mathbf{R})(\mathbf{b})_\beta(\mathbf{b})_\gamma(\mathbf{b})_\delta(\mathbf{b})_\epsilon(\mathbf{b})_\zeta\Bigg\} \\
& + \frac{1}{2!}\sum_{\alpha\beta}Q_{\alpha\beta}\Bigg\{\phi_{\alpha\beta}(\mathbf{R}) + \sum_\gamma\phi_{\alpha\beta\gamma}(\mathbf{R})(\mathbf{b})_\gamma
\end{aligned}$$

$$
\begin{aligned}
& + \frac{1}{2!}\sum_{\gamma\delta}\phi_{\alpha\beta\gamma\delta}(\mathbf{R})(\mathbf{b})_\gamma(\mathbf{b})_\delta \\
& + \frac{1}{3!}\sum_{\gamma\delta\epsilon}\phi_{\alpha\beta\gamma\delta\epsilon}(\mathbf{R})(\mathbf{b})_\gamma(\mathbf{b})_\delta(\mathbf{b})_\epsilon \\
& \left. + \frac{1}{4!}\sum_{\gamma\delta\epsilon\zeta}\phi_{\alpha\beta\gamma\delta\epsilon\zeta}(\mathbf{R})(\mathbf{b})_\gamma(\mathbf{b})_\delta(\mathbf{b})_\epsilon(\mathbf{b})_\zeta\right\} \\
& - \frac{1}{3!}\sum_{\alpha\beta\gamma}O_{\alpha\beta\gamma}\left\{\phi_{\alpha\beta\gamma}(\mathbf{R}) + \sum_{\delta}\phi_{\alpha\beta\gamma\delta}(\mathbf{R})(\mathbf{b})_\delta\right. \\
& + \frac{1}{2!}\sum_{\delta\epsilon}\phi_{\alpha\beta\gamma\delta\epsilon}(\mathbf{R})(\mathbf{b})_\delta(\mathbf{b})_\epsilon \\
& \left. + \frac{1}{3!}\sum_{\delta\epsilon\zeta}\phi_{\alpha\beta\gamma\delta\epsilon\zeta}(\mathbf{R})(\mathbf{b})_\delta(\mathbf{b})_\epsilon(\mathbf{b})_\zeta\right\} \\
& + \frac{1}{4!}\sum_{\alpha\beta\gamma\delta}H_{\alpha\beta\gamma\delta}\left\{\phi_{\alpha\beta\gamma\delta}(\mathbf{R}) + \sum_{\epsilon}\phi_{\alpha\beta\gamma\delta\epsilon}(\mathbf{R})(\mathbf{b})_\epsilon\right. \\
& \left. + \frac{1}{2!}\sum_{\epsilon\zeta}\phi_{\alpha\beta\gamma\delta\epsilon\zeta}(\mathbf{R})(\mathbf{b})_\epsilon(\mathbf{b})_\zeta\right\} \\
& - \frac{1}{5!}\sum_{\alpha\beta\gamma\delta\epsilon}T_{\alpha\beta\gamma\delta\epsilon}\left\{\phi_{\alpha\beta\gamma\delta\epsilon}(\mathbf{R}) + \sum_{\zeta}\phi_{\alpha\beta\gamma\delta\epsilon\zeta}(\mathbf{R})(\mathbf{b})_\zeta\right\} \\
& + \frac{1}{6!}\sum_{\alpha\beta\gamma\delta\epsilon\zeta}U_{\alpha\beta\gamma\delta\epsilon\zeta}\left\{\phi_{\alpha\beta\gamma\delta\epsilon\zeta}(\mathbf{R})\right\} \qquad (12) \\
= \; & \Psi(\mathbf{R}) + \sum_{\alpha}\Psi_\alpha(\mathbf{R})(\mathbf{b})_\alpha + \sum_{\alpha\beta}\Psi_{\alpha\beta}(\mathbf{R})(\mathbf{b})_\alpha(\mathbf{b})_\beta + \sum_{\alpha\beta\gamma}\Psi_{\alpha\beta\gamma}(\mathbf{R})(\mathbf{b})_\alpha(\mathbf{b})_\beta(\mathbf{b})_\gamma \\
& + \sum_{\alpha\beta\gamma\delta}\Psi_{\alpha\beta\gamma\delta}(\mathbf{R})(\mathbf{b})_\alpha(\mathbf{b})_\beta(\mathbf{b})_\gamma(\mathbf{b})_\delta + \sum_{\alpha\beta\gamma\delta\epsilon}\Psi_{\alpha\beta\gamma\delta\epsilon}(\mathbf{R})(\mathbf{b})_\alpha(\mathbf{b})_\beta(\mathbf{b})_\gamma(\mathbf{b})_\delta(\mathbf{b})_\epsilon \\
& + \sum_{\alpha\beta\gamma\delta\epsilon\zeta}\Psi_{\alpha\beta\gamma\delta\epsilon\zeta}(\mathbf{R})(\mathbf{b})_\alpha(\mathbf{b})_\beta(\mathbf{b})_\gamma(\mathbf{b})_\delta(\mathbf{b})_\epsilon(\mathbf{b})_\zeta, \qquad (13)
\end{aligned}
$$

where

$$
\begin{aligned}
\Psi(\mathbf{R}) &= M\phi(\mathbf{R}) - \sum_{\alpha}D_\alpha\phi_\alpha(\mathbf{R}) + \frac{1}{2!}\sum_{\alpha\beta}Q_{\alpha\beta}\phi_{\alpha\beta}(\mathbf{R}) - \frac{1}{3!}\sum_{\alpha\beta\gamma}O_{\alpha\beta\gamma}\phi_{\alpha\beta\gamma}(\mathbf{R}) \\
&\quad + \frac{1}{4!}\sum_{\alpha\beta\gamma\delta}H_{\alpha\beta\gamma\delta}\phi_{\alpha\beta\gamma\delta}(\mathbf{R}) - \frac{1}{5!}\sum_{\alpha\beta\gamma\delta\epsilon}T_{\alpha\beta\gamma\delta\epsilon}\phi_{\alpha\beta\gamma\delta\epsilon}(\mathbf{R}) \\
&\quad + \frac{1}{6!}\sum_{\alpha\beta\gamma\delta\epsilon\zeta}U_{\alpha\beta\gamma\delta\epsilon\zeta}\phi_{\alpha\beta\gamma\delta\epsilon\zeta}(\mathbf{R}), \qquad (14) \\
\Psi_\alpha(\mathbf{R}) &= M\phi_\alpha(\mathbf{R}) - \sum_{\beta}D_\beta\phi_{\alpha\beta}(\mathbf{R}) + \frac{1}{2}\sum_{\beta\gamma}Q_{\beta\gamma}\phi_{\alpha\beta\gamma}(\mathbf{R}) - \frac{1}{6}\sum_{\beta\gamma\delta}O_{\beta\gamma\delta}\phi_{\alpha\beta\gamma\delta}(\mathbf{R}) \\
&\quad + \frac{1}{24}\sum_{\beta\gamma\delta\epsilon}H_{\beta\gamma\delta\epsilon}\phi_{\alpha\beta\gamma\delta\epsilon}(\mathbf{R}) - \frac{1}{120}\sum_{\beta\gamma\delta\epsilon\zeta}T_{\beta\gamma\delta\epsilon\zeta}\phi_{\alpha\beta\gamma\delta\epsilon\zeta}(\mathbf{R}), \qquad (15) \\
\Psi_{\alpha\beta}(\mathbf{R}) &= \frac{1}{2}M\phi_{\alpha\beta}(\mathbf{R}) - \frac{1}{2}\sum_{\gamma}D_\gamma\phi_{\alpha\beta\gamma}(\mathbf{R}) + \frac{1}{4}\sum_{\gamma\delta}Q_{\gamma\delta}\phi_{\alpha\beta\gamma\delta}(\mathbf{R})
\end{aligned}
$$

$$
\begin{aligned}
& -\frac{1}{12}\sum_{\gamma\delta\epsilon} O_{\gamma\delta\epsilon}\phi_{\alpha\beta\gamma\delta\epsilon}(\mathbf{R}) + \frac{1}{48}\sum_{\gamma\delta\epsilon\zeta} H_{\gamma\delta\epsilon\zeta}\phi_{\alpha\beta\gamma\delta\epsilon\zeta}(\mathbf{R}), && (16)\\
\Psi_{\alpha\beta\gamma}(\mathbf{R}) &= \frac{1}{6}M\phi_{\alpha\beta\gamma}(\mathbf{R}) - \frac{1}{6}\sum_{\delta} D_\delta\phi_{\alpha\beta\gamma\delta}(\mathbf{R}) + \frac{1}{12}\sum_{\delta\epsilon} Q_{\delta\epsilon}\phi_{\alpha\beta\gamma\delta\epsilon}(\mathbf{R})\\
& -\frac{1}{36}\sum_{\delta\epsilon\zeta} O_{\delta\epsilon\zeta}\phi_{\alpha\beta\gamma\delta\epsilon\zeta}(\mathbf{R}), && (17)\\
\Psi_{\alpha\beta\gamma\delta}(\mathbf{R}) &= \frac{1}{24}M\phi_{\alpha\beta\gamma\delta}(\mathbf{R}) - \frac{1}{24}\sum_{\epsilon} D_\epsilon\phi_{\alpha\beta\gamma\delta\epsilon}(\mathbf{R}) + \frac{1}{48}\sum_{\epsilon\zeta} Q_{\epsilon\zeta}\phi_{\alpha\beta\gamma\delta\epsilon\zeta}(\mathbf{R}), && (18)\\
\Psi_{\alpha\beta\gamma\delta\epsilon}(\mathbf{R}) &= \frac{1}{120}M\phi_{\alpha\beta\gamma\delta\epsilon}(\mathbf{R}) - \frac{1}{120}\sum_{\zeta} D_\zeta\phi_{\alpha\beta\gamma\delta\epsilon\zeta}(\mathbf{R}), && (19)\\
\Psi_{\alpha\beta\gamma\delta\epsilon\zeta}(\mathbf{R}) &= \frac{1}{720}M\phi_{\alpha\beta\gamma\delta\epsilon\zeta}(\mathbf{R}). && (20)
\end{aligned}
$$

Here each term of mutipole expansions is expanded until the sixth derivatives of ϕ emerge.

2.1.3 Derivatives of Yukawa potential

The derivatives of pairwise interaction potential $\phi(r)$ in Cartesian coordinates are generally expressed as

$$\phi_\alpha(\mathbf{r}) = \frac{\partial\phi}{\partial r_\alpha} = \frac{\partial\phi}{\partial r}\frac{r_\alpha}{r}, \tag{21}$$

$$\phi_{\alpha\beta}(\mathbf{r}) = \left(\frac{\partial^2\phi}{\partial r^2} - \frac{1}{r}\frac{\partial\phi}{\partial r}\right)\frac{r_\alpha}{r}\frac{r_\beta}{r} + \frac{1}{r}\frac{\partial\phi}{\partial r}\delta_{\alpha\beta}, \tag{22}$$

$$
\begin{aligned}
\phi_{\alpha\beta\gamma}(\mathbf{r}) &= \left(\frac{\partial^3\phi}{\partial r^3} - \frac{3}{r}\frac{\partial^2\phi}{\partial r^2} + \frac{3}{r^2}\frac{\partial\phi}{\partial r}\right)\frac{r_\alpha}{r}\frac{r_\beta}{r}\frac{r_\gamma}{r}\\
&+\frac{1}{r}\left(\frac{\partial^2\phi}{\partial r^2} - \frac{1}{r}\frac{\partial\phi}{\partial r}\right)\left(\frac{r_\gamma}{r}\delta_{\alpha\beta} + \frac{r_\beta}{r}\delta_{\gamma\alpha} + \frac{r_\alpha}{r}\delta_{\beta\gamma}\right), \qquad (23)
\end{aligned}
$$

$$
\begin{aligned}
\phi_{\alpha\beta\gamma\delta}(\mathbf{r}) &= \left(\frac{\partial^4\phi}{\partial r^4} - \frac{6}{r}\frac{\partial^3\phi}{\partial r^3} + \frac{15}{r^2}\frac{\partial^2\phi}{\partial r^2} - \frac{15}{r^3}\frac{\partial\phi}{\partial r}\right)\frac{r_\alpha}{r}\frac{r_\beta}{r}\frac{r_\gamma}{r}\frac{r_\delta}{r}\\
&+\frac{1}{r}\left(\frac{\partial^3\phi}{\partial r^3} - \frac{3}{r}\frac{\partial^2\phi}{\partial r^2} + \frac{3}{r^2}\frac{\partial\phi}{\partial r}\right)\\
&\times\left(\frac{r_\beta}{r}\frac{r_\gamma}{r}\delta_{\alpha\delta} + \frac{r_\alpha}{r}\frac{r_\gamma}{r}\delta_{\beta\delta} + \frac{r_\alpha}{r}\frac{r_\beta}{r}\delta_{\gamma\delta} + \frac{r_\gamma}{r}\frac{r_\delta}{r}\delta_{\alpha\beta} + \frac{r_\beta}{r}\frac{r_\delta}{r}\delta_{\alpha\gamma} + \frac{r_\alpha}{r}\frac{r_\delta}{r}\delta_{\beta\gamma}\right)\\
&+\frac{1}{r^2}\left(\frac{\partial^2\phi}{\partial r^2} - \frac{1}{r}\frac{\partial\phi}{\partial r}\right)\left(\delta_{\gamma\delta}\delta_{\alpha\beta} + \delta_{\beta\delta}\delta_{\alpha\gamma} + \delta_{\alpha\delta}\delta_{\beta\gamma}\right), \qquad (24)
\end{aligned}
$$

$$
\begin{aligned}
\phi_{\alpha\beta\gamma\delta\epsilon}(\mathbf{r}) &= \left(\frac{\partial^5\phi}{\partial r^5} - \frac{10}{r}\frac{\partial^4\phi}{\partial r^4} + \frac{45}{r^2}\frac{\partial^3\phi}{\partial r^3} - \frac{105}{r^3}\frac{\partial^2\phi}{\partial r^2} + \frac{105}{r^4}\frac{\partial\phi}{\partial r}\right)\frac{r_\alpha}{r}\frac{r_\beta}{r}\frac{r_\gamma}{r}\frac{r_\delta}{r}\frac{r_\epsilon}{r}\\
&+\frac{1}{r}\left(\frac{\partial^4\phi}{\partial r^4} - \frac{6}{r}\frac{\partial^3\phi}{\partial r^3} + \frac{15}{r^2}\frac{\partial^2\phi}{\partial r^2} - \frac{15}{r^3}\frac{\partial\phi}{\partial r}\right)
\end{aligned}
$$

$$\times\left(\frac{r_\beta}{r}\frac{r_\gamma}{r}\frac{r_\epsilon}{r}\delta_{\alpha\delta}+\frac{r_\alpha}{r}\frac{r_\gamma}{r}\frac{r_\epsilon}{r}\delta_{\beta\delta}+\frac{r_\alpha}{r}\frac{r_\beta}{r}\frac{r_\epsilon}{r}\delta_{\gamma\delta}+\frac{r_\gamma}{r}\frac{r_\delta}{r}\frac{r_\epsilon}{r}\delta_{\alpha\beta}+\frac{r_\beta}{r}\frac{r_\delta}{r}\frac{r_\epsilon}{r}\delta_{\alpha\gamma}\right.$$
$$\left.+\frac{r_\alpha}{r}\frac{r_\delta}{r}\frac{r_\epsilon}{r}\delta_{\beta\gamma}+\frac{r_\beta}{r}\frac{r_\gamma}{r}\frac{r_\delta}{r}\delta_{\alpha\epsilon}+\frac{r_\alpha}{r}\frac{r_\gamma}{r}\frac{r_\delta}{r}\delta_{\beta\epsilon}+\frac{r_\alpha}{r}\frac{r_\beta}{r}\frac{r_\delta}{r}\delta_{\gamma\epsilon}+\frac{r_\alpha}{r}\frac{r_\beta}{r}\frac{r_\gamma}{r}\delta_{\delta\epsilon}\right)$$
$$+\frac{1}{r^2}\left(\frac{\partial^3\phi}{\partial r^3}-\frac{3}{r}\frac{\partial^2\phi}{\partial r^2}+\frac{3}{r^2}\frac{\partial\phi}{\partial r}\right)$$
$$\times\left\{(\delta_{\beta\delta}\delta_{\gamma\epsilon}+\delta_{\gamma\delta}\delta_{\beta\epsilon}+\delta_{\beta\gamma}\delta_{\delta\epsilon})\frac{r_\alpha}{r}+(\delta_{\alpha\delta}\delta_{\gamma\epsilon}+\delta_{\gamma\delta}\delta_{\alpha\epsilon}+\delta_{\alpha\gamma}\delta_{\delta\epsilon})\frac{r_\beta}{r}\right.$$
$$+(\delta_{\alpha\delta}\delta_{\beta\epsilon}+\delta_{\beta\delta}\delta_{\alpha\epsilon}+\delta_{\alpha\beta}\delta_{\delta\epsilon})\frac{r_\gamma}{r}+(\delta_{\alpha\beta}\delta_{\gamma\epsilon}+\delta_{\alpha\gamma}\delta_{\beta\epsilon}+\delta_{\beta\gamma}\delta_{\alpha\epsilon})\frac{r_\delta}{r}$$
$$\left.+(\delta_{\gamma\delta}\delta_{\alpha\beta}+\delta_{\beta\delta}\delta_{\alpha\gamma}+\delta_{\alpha\delta}\delta_{\beta\gamma})\frac{r_\epsilon}{r}\right\}, \qquad (25)$$

$$\phi_{\alpha\beta\gamma\delta\epsilon\zeta}(\mathbf{r}) = \left(\frac{\partial^6\phi}{\partial r^6}-\frac{15}{r}\frac{\partial^5\phi}{\partial r^5}+\frac{105}{r^2}\frac{\partial^4\phi}{\partial r^4}-\frac{420}{r^3}\frac{\partial^3\phi}{\partial r^3}+\frac{945}{r^4}\frac{\partial^2\phi}{\partial r^2}-\frac{945}{r^5}\frac{\partial\phi}{\partial r}\right)\frac{r_\alpha}{r}\frac{r_\beta}{r}\frac{r_\gamma}{r}\frac{r_\delta}{r}\frac{r_\epsilon}{r}\frac{r_\zeta}{r}$$
$$+\frac{1}{r}\left(\frac{\partial^5\phi}{\partial r^5}-\frac{10}{r}\frac{\partial^4\phi}{\partial r^4}+\frac{45}{r^2}\frac{\partial^3\phi}{\partial r^3}-\frac{105}{r^3}\frac{\partial^2\phi}{\partial r^2}+\frac{105}{r^4}\frac{\partial\phi}{\partial r}\right)$$
$$\times\left(\frac{r_\beta}{r}\frac{r_\gamma}{r}\frac{r_\delta}{r}\frac{r_\epsilon}{r}\delta_{\alpha\zeta}+\frac{r_\alpha}{r}\frac{r_\gamma}{r}\frac{r_\delta}{r}\frac{r_\epsilon}{r}\delta_{\beta\zeta}+\frac{r_\alpha}{r}\frac{r_\beta}{r}\frac{r_\delta}{r}\frac{r_\epsilon}{r}\delta_{\gamma\zeta}+\frac{r_\alpha}{r}\frac{r_\beta}{r}\frac{r_\gamma}{r}\frac{r_\delta}{r}\delta_{\epsilon\zeta}\right.$$
$$+\frac{r_\alpha}{r}\frac{r_\beta}{r}\frac{r_\gamma}{r}\frac{r_\epsilon}{r}\delta_{\delta\zeta}+\frac{r_\beta}{r}\frac{r_\gamma}{r}\frac{r_\epsilon}{r}\frac{r_\zeta}{r}\delta_{\alpha\delta}+\frac{r_\alpha}{r}\frac{r_\gamma}{r}\frac{r_\epsilon}{r}\frac{r_\zeta}{r}\delta_{\beta\delta}+\frac{r_\alpha}{r}\frac{r_\beta}{r}\frac{r_\epsilon}{r}\frac{r_\zeta}{r}\delta_{\gamma\delta}$$
$$+\frac{r_\gamma}{r}\frac{r_\delta}{r}\frac{r_\epsilon}{r}\frac{r_\zeta}{r}\delta_{\alpha\beta}+\frac{r_\beta}{r}\frac{r_\delta}{r}\frac{r_\epsilon}{r}\frac{r_\zeta}{r}\delta_{\alpha\gamma}+\frac{r_\alpha}{r}\frac{r_\delta}{r}\frac{r_\epsilon}{r}\frac{r_\zeta}{r}\delta_{\beta\gamma}+\frac{r_\beta}{r}\frac{r_\gamma}{r}\frac{r_\delta}{r}\frac{r_\zeta}{r}\delta_{\alpha\epsilon}$$
$$\left.+\frac{r_\alpha}{r}\frac{r_\gamma}{r}\frac{r_\delta}{r}\frac{r_\zeta}{r}\delta_{\beta\epsilon}+\frac{r_\alpha}{r}\frac{r_\beta}{r}\frac{r_\delta}{r}\frac{r_\zeta}{r}\delta_{\gamma\epsilon}+\frac{r_\alpha}{r}\frac{r_\beta}{r}\frac{r_\gamma}{r}\frac{r_\zeta}{\delta}\,\delta_{\epsilon}\right)$$
$$+\frac{1}{r^2}\left(\frac{\partial^4\phi}{\partial r^4}-\frac{6}{r}\frac{\partial^3\phi}{\partial r^3}+\frac{15}{r^2}\frac{\partial^2\phi}{\partial r^2}-\frac{15}{r^3}\frac{\partial\phi}{\partial r}\right)$$
$$\times\left((\delta_{\alpha\delta}\delta_{\beta\zeta}+\delta_{\beta\delta}\delta_{\alpha\zeta}+\delta_{\alpha\beta}\delta_{\delta\zeta})\frac{r_\gamma}{r}\frac{r_\epsilon}{r}+(\delta_{\alpha\delta}\delta_{\gamma\zeta}+\delta_{\gamma\delta}\delta_{\alpha\zeta}+\delta_{\alpha\gamma}\delta_{\delta\zeta})\frac{r_\beta}{r}\frac{r_\epsilon}{r}\right.$$
$$+(\delta_{\beta\delta}\delta_{\gamma\zeta}+\delta_{\gamma\delta}\delta_{\beta\zeta}+\delta_{\beta\gamma}\delta_{\delta\zeta})\frac{r_\alpha}{r}\frac{r_\epsilon}{r}+(\delta_{\alpha\delta}\delta_{\epsilon\zeta}+\delta_{\alpha\epsilon}\delta_{\delta\zeta}+\delta_{\delta\epsilon}\delta_{\alpha\zeta})\frac{r_\beta}{r}\frac{r_\gamma}{r}$$
$$+(\delta_{\beta\delta}\delta_{\epsilon\zeta}+\delta_{\beta\epsilon}\delta_{\delta\zeta}+\delta_{\delta\epsilon}\delta_{\beta\zeta})\frac{r_\alpha}{r}\frac{r_\gamma}{r}+(\delta_{\alpha\beta}\delta_{\gamma\zeta}+\delta_{\alpha\gamma}\delta_{\beta\zeta}+\delta_{\beta\gamma}\delta_{\alpha\zeta})\frac{r_\delta}{r}\frac{r_\epsilon}{r}$$
$$+(\delta_{\gamma\delta}\delta_{\epsilon\zeta}+\delta_{\gamma\epsilon}\delta_{\delta\zeta}+\delta_{\delta\epsilon}\delta_{\gamma\zeta})\frac{r_\alpha}{r}\frac{r_\beta}{r}+(\delta_{\alpha\beta}\delta_{\epsilon\zeta}+\delta_{\alpha\epsilon}\delta_{\beta\zeta}+\delta_{\beta\epsilon}\delta_{\alpha\zeta})\frac{r_\gamma}{r}\frac{r_\delta}{r}$$
$$+(\delta_{\alpha\gamma}\delta_{\epsilon\zeta}+\delta_{\alpha\epsilon}\delta_{\gamma\zeta}+\delta_{\gamma\epsilon}\delta_{\alpha\zeta})\frac{r_\beta}{r}\frac{r_\delta}{r}+(\delta_{\beta\gamma}\delta_{\epsilon\zeta}+\delta_{\beta\epsilon}\delta_{\gamma\zeta}+\delta_{\gamma\epsilon}\delta_{\beta\zeta})\frac{r_\alpha}{r}\frac{r_\delta}{r}$$
$$+(\delta_{\beta\delta}\delta_{\gamma\epsilon}+\delta_{\gamma\delta}\delta_{\beta\epsilon}+\delta_{\beta\gamma}\delta_{\delta\epsilon})\frac{r_\alpha}{r}\frac{r_\zeta}{r}+(\delta_{\alpha\delta}\delta_{\gamma\epsilon}+\delta_{\gamma\delta}\delta_{\alpha\epsilon}+\delta_{\alpha\gamma}\delta_{\delta\epsilon})\frac{r_\beta}{r}\frac{r_\zeta}{r}$$
$$+(\delta_{\alpha\delta}\delta_{\beta\epsilon}+\delta_{\beta\delta}\delta_{\alpha\epsilon}+\delta_{\alpha\beta}\delta_{\delta\epsilon})\frac{r_\gamma}{r}\frac{r_\zeta}{r}+(\delta_{\alpha\beta}\delta_{\gamma\epsilon}+\delta_{\alpha\gamma}\delta_{\beta\epsilon}+\delta_{\beta\gamma}\delta_{\alpha\epsilon})\frac{r_\delta}{r}\frac{r_\zeta}{r}$$
$$\left.+(\delta_{\gamma\delta}\delta_{\alpha\beta}+\delta_{\beta\delta}\delta_{\alpha\gamma}+\delta_{\alpha\delta}\delta_{\beta\gamma})\frac{r_\epsilon}{r}\frac{r_\zeta}{r}\right)$$
$$+\frac{1}{r^3}\left(\frac{\partial^3\phi}{\partial r^3}-\frac{3}{r}\frac{\partial^2\phi}{\partial r^2}+\frac{3}{r^2}\frac{\partial\phi}{\partial r}\right)$$
$$\times(\delta_{\beta\delta}\delta_{\gamma\epsilon}\delta_{\alpha\zeta}+\delta_{\gamma\delta}\delta_{\beta\epsilon}\delta_{\alpha\zeta}+\delta_{\beta\gamma}\delta_{\delta\epsilon}\delta_{\alpha\zeta}+\delta_{\alpha\delta}\delta_{\gamma\epsilon}\delta_{\beta\zeta}+\delta_{\gamma\delta}\delta_{\alpha\epsilon}\delta_{\beta\zeta}+\delta_{\alpha\gamma}\delta_{\delta\epsilon}\delta_{\beta\zeta}$$
$$+\delta_{\alpha\delta}\delta_{\beta\epsilon}\delta_{\gamma\zeta}+\delta_{\beta\delta}\delta_{\alpha\epsilon}\delta_{\gamma\zeta}+\delta_{\alpha\beta}\delta_{\delta\epsilon}\delta_{\gamma\zeta}+\delta_{\alpha\beta}\delta_{\gamma\epsilon}\delta_{\delta\zeta}+\delta_{\alpha\gamma}\delta_{\beta\epsilon}\delta_{\delta\zeta}+\delta_{\beta\gamma}\delta_{\alpha\epsilon}\delta_{\delta\zeta}$$
$$+\delta_{\gamma\delta}\delta_{\alpha\beta}\delta_{\epsilon\zeta}+\delta_{\beta\delta}\delta_{\alpha\gamma}\delta_{\epsilon\zeta}+\delta_{\alpha\delta}\delta_{\beta\gamma}\delta_{\epsilon\zeta}), \qquad (26)$$

where $\delta_{\alpha\beta}$ is Kronecker delta symbol. (if $\alpha = \beta, \delta_{\alpha\beta} = 1$, and otherwise $\delta_{\alpha\beta} = 0$).

In the case of Yukawa potential

$$\phi(r) = \frac{1}{r}\exp(-\kappa r), \tag{27}$$

the terms in parentheses in the expressions above are

$$\frac{\partial\phi}{\partial r} = \left(-\frac{1}{r} - \kappa\right)\phi(r), \tag{28}$$

$$\frac{\partial^2\phi}{\partial r^2} - \frac{1}{r}\frac{\partial\phi}{\partial r} = \left(3\frac{1}{r^2} + 3\frac{\kappa}{r} + \kappa^2\right)\phi(r), \tag{29}$$

$$\frac{\partial^3\phi}{\partial r^3} - \frac{3}{r}\frac{\partial^2\phi}{\partial r^2} + \frac{3}{r^2}\frac{\partial\phi}{\partial r} = \left(-15\frac{1}{r^3} - 15\frac{\kappa}{r^2} - 6\frac{\kappa^2}{r} - \kappa^3\right)\phi(r), \tag{30}$$

$$\begin{aligned}&\frac{\partial^4\phi}{\partial r^4} - \frac{6}{r}\frac{\partial^3\phi}{\partial r^3} + \frac{15}{r^2}\frac{\partial^2\phi}{\partial r^2} - \frac{15}{r^3}\frac{\partial\phi}{\partial r} \\ &= \left(105\frac{1}{r^4} + 105\frac{\kappa}{r^3} + 45\frac{\kappa^2}{r^2} + 10\frac{\kappa^3}{r} + \kappa^4\right)\phi(r),\end{aligned} \tag{31}$$

$$\begin{aligned}&\frac{\partial^5\phi}{\partial r^5} - \frac{10}{r}\frac{\partial^4\phi}{\partial r^4} + \frac{45}{r^2}\frac{\partial^3\phi}{\partial r^3} - \frac{105}{r^3}\frac{\partial^2\phi}{\partial r^2} + \frac{105}{r^4}\frac{\partial\phi}{\partial r} \\ &= \left(-945\frac{1}{r^5} - 945\frac{\kappa}{r^4} - 420\frac{\kappa^2}{r^3} - 105\frac{\kappa^3}{r^2} - 15\frac{\kappa^4}{r} - \kappa^5\right)\phi(r),\end{aligned} \tag{32}$$

$$\begin{aligned}&\frac{\partial^6\phi}{\partial r^6} - \frac{15}{r}\frac{\partial^5\phi}{\partial r^5} + \frac{105}{r^2}\frac{\partial^4\phi}{\partial r^4} - \frac{420}{r^3}\frac{\partial^3\phi}{\partial r^3} + \frac{945}{r^4}\frac{\partial^2\phi}{\partial r^2} - \frac{945}{r^5}\frac{\partial\phi}{\partial r} \\ &= \left(10395\frac{1}{r^6} + 10395\frac{\kappa}{r^5} + 4725\frac{\kappa^2}{r^4} + 1260\frac{\kappa^3}{r^3} + 210\frac{\kappa^4}{r^2} + 21\frac{\kappa^4}{r} + \kappa^6\right)\phi(r).\end{aligned} \tag{33}$$

2.2 Algorithm

We here describe the algorithm of the fast multipole method. In this method, the simulation box is hierarchically divided into small spatial regions (Fig. 2). The simulation box is first divided into eight cubic boxes. Each of eight boxes is subdivided into eight boxes. This procedure is repeated until the smallest box contains only a small certain number of particles. It is essential for $O(N)$ scaling that the number of particles per box is independent of the total number of particles. After l-times subdivision (at level l), we have equivalent 8^l boxes. The eight boxes are called *child* for a original box and the original box is called *parent* for its eight children's boxes.

Each box corresponds to a local region in Fig. 1. When evaluating the potential due to distant particles, the different level boxes are used. In Fig. 3, we show an example of boxes interacting with particles within a box. The hatched box near the center of the simulation box is the box where the potential is evaluated. As the distance from the hatched box increases, the size of the box becomes larger. Which level boxes are used is determined hierarchically and expressed by using the term *interaction list.* In Fig. 3, we shows the interaction list of a box at level 4 (leaf level). For the hatched box, shaded boxes are members of its interaction list. The

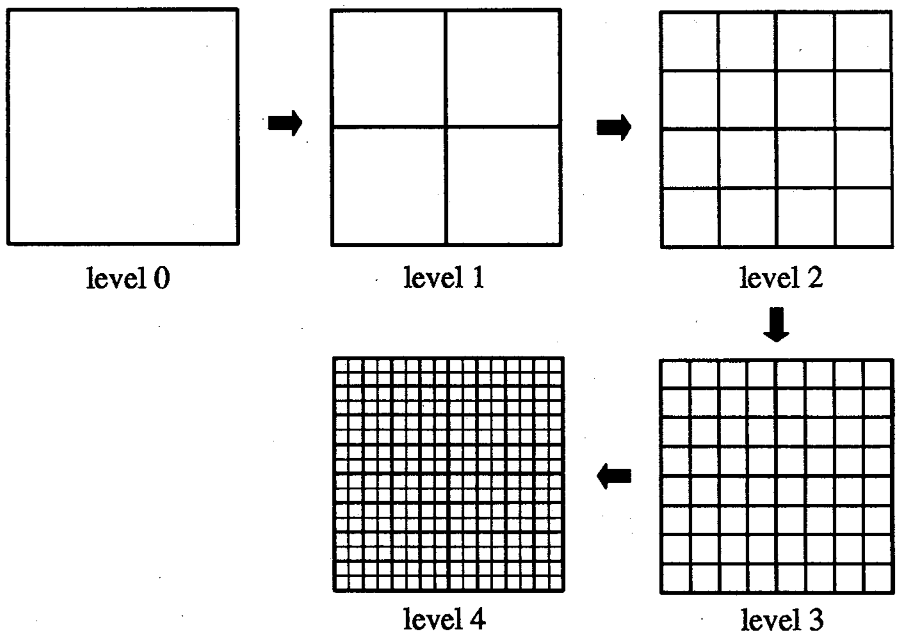


Figure 2: Division of the simulation box. The box at level 0 is equivalent to the simulation box.

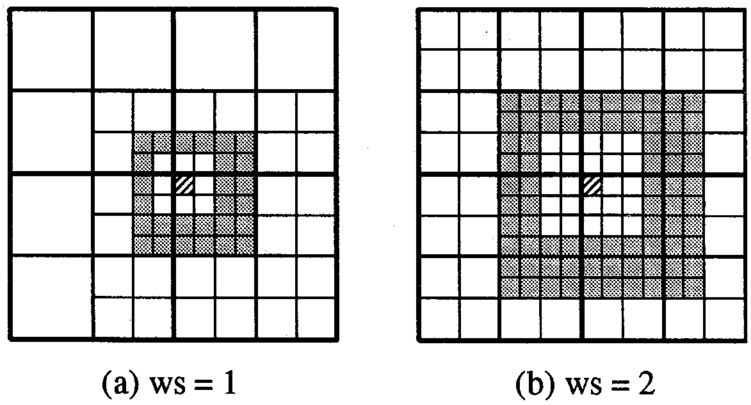


Figure 3: Schematic diagrams showing interacting boxes. As the distance from the hatched box, where the potential is evaluated, increases, the size of interacting boxes becomes larger. For the hatched box, the shaded boxes are members of its interaction list. Interaction list is a list of boxes that are well-separated from the current box, but not well-separated from its parent. For $ws = 1$, boxes separated by one box are considered to be well-separated and for $ws = 2$, boxes separated by two boxes are considered to be well-separated.

interaction list is a list of boxes which are well-separated from a box, but not well-separated from its parent. In Fig. 3 (a), the boxes separated by one box are considered to be well-separated. We denote this "well-separatedness" as $ws = 1$. While, in Fig. 3 (b), the boxes separated by two boxes are considered to be well-separated and we denote this as $ws = 2$. Using the term "interaction list", the list of boxes where distant particles reside is hierarchically expressed as "interaction list of current box + interaction list of its parent + interaction list of parent of its parent + $\cdots$". For each box at each level, there is a constant number of boxes in the interaction list.. For ws=1, there are maximum number of 189 boxes in the interaction list and 875 boxes for $ws = 2$.

The following is the flow for an MD step.

[Upward Pass]
In this step, for every box at every level, the moments of multipole expansions are evaluated about the center of the box. we show the flow of this step in Fig. 4. First, for all boxes at leaf level (level 4), the moments of multipole expansions are evaluated about the center of the box using Eq. (4). For coarser level boxes, the moments of multipole expansion are obtained from its children's moments by shifting the origin. (The mathematical expressions for origin shift are described later.) Therefore, once we evaluate the multipole moments at leaf level (level 4), we ascend from level 4 to level 2, evaluating the moments at coarser level by shifting the origin.

[Downward Pass]
In this step, the potential at a given point is evaluated. First, this step evaluate the Taylor expansion of the potential due to distant particles, $\Phi_{distant}$, for all boxes at leaf level. The flow of this step is shown in Fig. 5. The current box at each level, which contain the leaf level box where the potential is evaluated, is denoted by thick line square. The Taylor expansion of the potential at leaf level, $\Phi^{(leaf)}$ [$=\Phi_{distant}$], is obtained hierarchically as

$$\Phi^{(2)} = \Phi^{(2)}_{list}, \tag{34}$$

$$\Phi^{(3)} = \Phi^{(3)}_{list} + \Phi^{(3)}_{outside}, \quad \Phi^{(3)}_{outside} = \Phi^{(2)} \text{ with shifted origin}, \tag{35}$$

$$\cdots$$

$$\Phi^{(l)} = \Phi^{(l)}_{list} + \Phi^{(l)}_{outside}, \quad \Phi^{(l)}_{outside} = \Phi^{(l-1)} \text{ with shifted origin}, \tag{36}$$

$$\cdots$$

$$\Phi^{(leaf)} = \Phi^{(leaf)}_{list} + \Phi^{(leaf)}_{outside}, \quad \Phi^{(leaf)}_{outside} = \Phi^{(leaf-1)} \text{ with shifted origin}. \tag{37}$$

Here, $\Phi^{(l)}$ is the Taylor expansion of the potential about the center of current box at level l due to particles outside the current box's nearest neighbors. $\Phi^{(l)}_{list}$ is the Taylor expansion of the potential due to particles in the interaction list of the current box at level l and obtained by using Eq. (13). $\Phi^{(l)}_{outside}$ is the Taylor expansion of the potential due to particles outside the parent box's nearest neighbors. The coefficients of the Taylor expansion $\{\Psi^{(l)}, \Psi^{(l)}_\alpha, \ldots\}$ can be obtained from those of parent box, $\{\Psi^{(l-1)}, \Psi^{(l-1)}_\alpha, \ldots\}$ by shifting the origin from parent box to the current box at level l. (The mathematical expressions for origin shift are described later.) While evaluating $\Phi^{(l)}$ about the center of each box at each level, we descend from level 2 to level 4 (leaf level).

Second, for all boxes at leaf level, the potential due to nearby particles, Φ_{near}, is calculated directly and added to the Taylor expansion of the potential due to distant particles, giving the potential due to all particles as

$$\Phi_{tot}(\mathbf{r}) = \sum_j^{n.n.} \frac{q_j}{|\mathbf{r} - \mathbf{r}_j|} \exp\left(\kappa|\mathbf{r} - \mathbf{r}_j|\right) + \Phi^{(leaf)}(\mathbf{r}), \tag{38}$$

where the summation is over particles within the leaf level box and its nearest neighbor boxes.

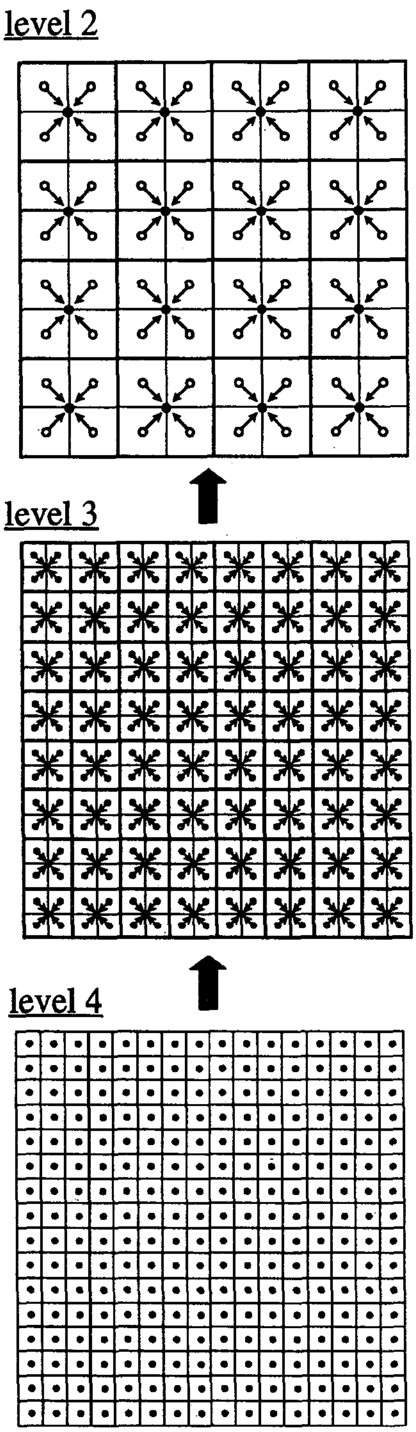


Figure 4: A schematic diagram showing the upward pass. The current box at each level is denoted by thick line square. Solid circles are the center of current boxes and open circles are the center of its children. Once we evaluate the moments at leaf level (level 4), we ascend from level 4 to level 2, evaluating the moments of multipole expansion about the center of current box at each level by shifting the origin.

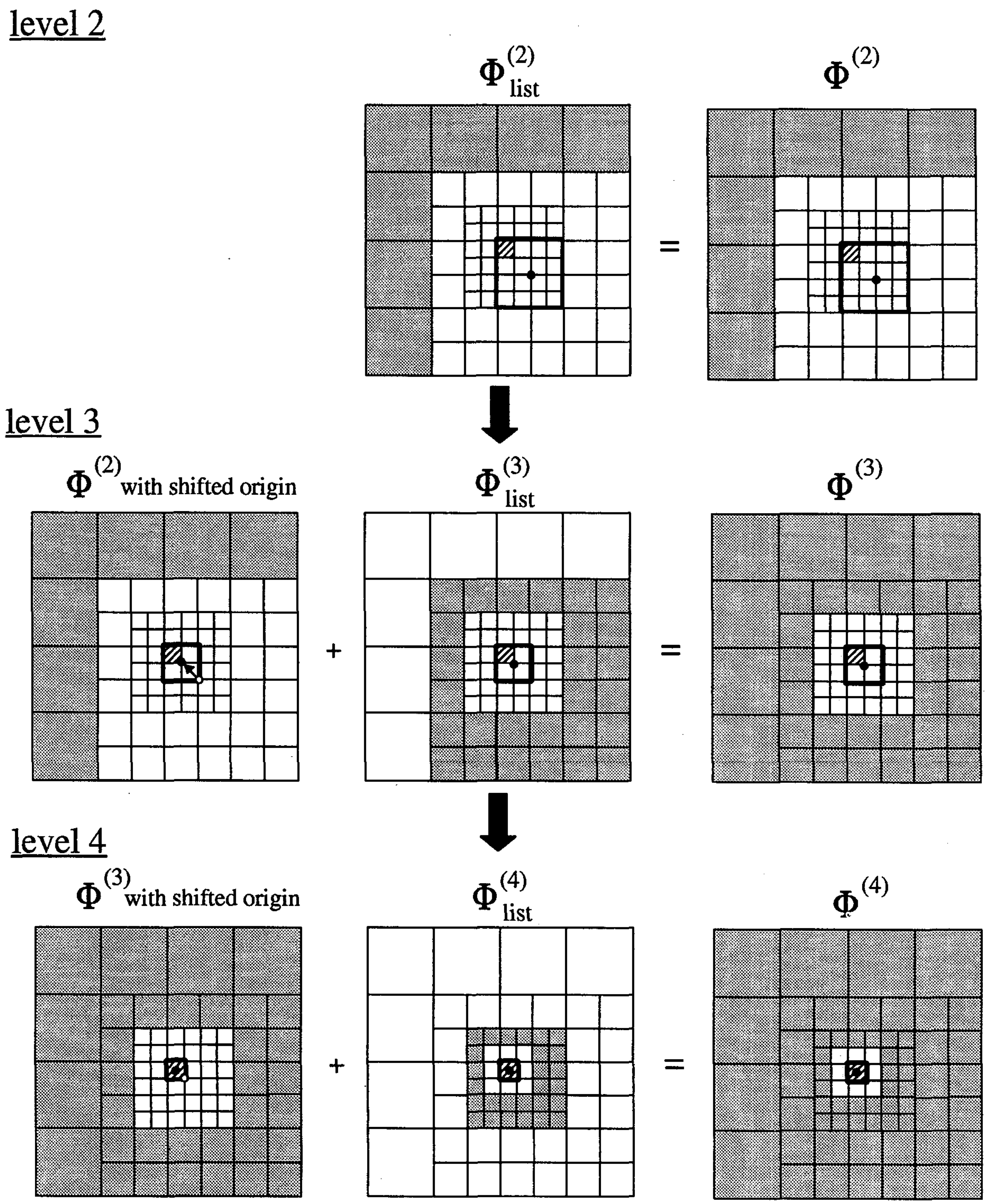


Figure 5: A schematic diagram showing the downward pass. The hatched box near the center of the simulation box is a leaf level box where the potential is evaluated. The current box at each level is denoted by thick line square. Solid circle is the origin (center) of the current box. Open circle is the origin of the current box's parent. Shaded boxes are boxes that are outside the current box and its nearest neighbors. We descend from level 2 to level 4 (leaf level), evaluating the Taylor expansion of the potential due to particles within shaded boxes about the center of current box.

[Numerical Integration]
The positions and the velocities of particles at next time step, $t+\Delta t$, are obtained by numerically integrating the equations of motion. In this process, we need to calculate the forces exerted on particles. Since we have the potential at a particle's position, the force is immediately obtained by the derivative. The force exerted on ith particle is given by

$$\begin{aligned}\mathbf{F}_i &= -q_i\frac{\partial}{\partial \mathbf{r}}\Phi_{tot}(\mathbf{r}_i) \\ &= q_i\sum_j^{n.n.} q_j\frac{\mathbf{r}_i-\mathbf{r}_j}{|\mathbf{r}_i-\mathbf{r}_j|^3}(1+\kappa|\mathbf{r}_i-\mathbf{r}_j|) - q_i\frac{\partial}{\partial \mathbf{r}}\Phi(\mathbf{r}_i), \end{aligned} \tag{39}$$

where

$$\begin{aligned}\frac{\partial}{\partial r_\alpha}\Phi(\mathbf{r}) &= \Psi_\alpha + 2\sum_\beta \Psi_{\alpha\beta}\mathbf{r}_\beta + 3\sum_{\beta\gamma}\Psi_{\alpha\beta\gamma}\mathbf{r}_\beta\mathbf{r}_\gamma \\ &+ 4\sum_{\beta\gamma\delta}\Psi_{\alpha\beta\gamma\delta}\mathbf{r}_\beta\mathbf{r}_\gamma\mathbf{r}_\delta + 5\sum_{\beta\gamma\delta\epsilon}\Psi_{\alpha\beta\gamma\delta\epsilon}\mathbf{r}_\beta\mathbf{r}_\gamma\mathbf{r}_\delta\mathbf{r}_\epsilon \\ &+ 6\sum_{\beta\gamma\delta\epsilon\zeta}\Psi_{\alpha\beta\gamma\delta\epsilon\zeta}\mathbf{r}_\beta\mathbf{r}_\gamma\mathbf{r}_\delta\mathbf{r}_\epsilon\mathbf{r}_\zeta .\end{aligned}$$

2.2.1 Origin Shift in Upward Path

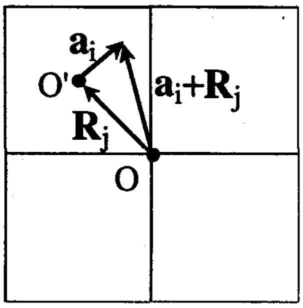


Figure 6: A schemetic diagram showing the origin shift in the upward pass. The symbol O is the origin (center) of the current box at level l and O' is the origin of its child's box at level $l+1$.

The multipole moments at level l, $\{M^{(l)}, D_\alpha^{(l)}, \ldots\}$, are obtained from its children's multipole moments at level $l+1$, $\{M^{(l+1)}, D_\alpha^{(l+1)}, \ldots\}$, by shifting the origin (Fig. 2.2.1).

$$M^{(l)} = \sum_{j=1}^{8}\sum_i q_{i(j)} = \sum_{j=1}^{8} M_{(j)}^{(l+1)}, \tag{40}$$

$$\begin{aligned}D_\alpha^{(l)} &= \sum_{j=1}^{8}\sum_i q_{i(j)}(\mathbf{a}_{i(j)}+\mathbf{R}_j)_\alpha \\ &= \sum_{j=1}^{8}\left\{D_{\alpha(j)}^{(l+1)} + (\mathbf{R}_j)_\alpha M_{(j)}^{(l+1)}\right\},\end{aligned} \tag{41}$$

$$Q_{\alpha\beta}^{(l)} = \sum_{j=1}^{8}\sum_i q_{i(j)}(\mathbf{a}_{i(j)}+\mathbf{R}_j)_\alpha(\mathbf{a}_{i(j)}+\mathbf{R}_j)_\beta$$

$$
\begin{aligned}
&= \sum_{j=1}^{8}\left\{Q^{(l+1)}_{\alpha\beta(j)} + (\mathbf{R}_j)_\beta D^{(l+1)}_{\alpha(j)} + (\mathbf{R}_j)_\alpha D^{(l+1)}_{\beta(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\beta M^{(l+1)}_{(j)}\right\}, \qquad (42)\\
O^{(l)}_{\alpha\beta\gamma} &= \sum_{j=1}^{8}\sum_i q_{i(j)}(\mathbf{a}_{i(j)}+\mathbf{R}_j)_\alpha(\mathbf{a}_{i(j)}+\mathbf{R}_j)_\beta(\mathbf{a}_{i(j)}+\mathbf{R}_j)_\gamma\\
&= \sum_{j=1}^{8}\left\{O^{(l+1)}_{\alpha\beta\gamma(j)} + (\mathbf{R}_j)_\gamma Q^{(l+1)}_{\alpha\beta(j)} + (\mathbf{R}_j)_\beta Q^{(l+1)}_{\alpha\gamma(j)} + (\mathbf{R}_j)_\alpha Q^{(l+1)}_{\beta\gamma(j)}\right.\\
&\quad + (\mathbf{R}_j)_\beta(\mathbf{R}_j)_\gamma D^{(l+1)}_{\alpha(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\gamma D^{(l+1)}_{\beta(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\beta D^{(l+1)}_{\gamma(j)}\\
&\quad \left. + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\beta(\mathbf{R}_j)_\gamma M^{(l+1)}_{(j)}\right\}, \qquad (43)\\
H^{(l)}_{\alpha\beta\gamma\delta} &= \sum_{j=1}^{8}\sum_i q_{i(j)}(\mathbf{a}_{i(j)}+\mathbf{R}_j)_\alpha(\mathbf{a}_{i(j)}+\mathbf{R}_j)_\beta(\mathbf{a}_{i(j)}+\mathbf{R}_j)_\gamma(\mathbf{a}_{i(j)}+\mathbf{R}_j)_\delta\\
&= \sum_{j=1}^{8}\left\{H^{(l+1)}_{\alpha\beta\gamma\delta(j)} + (\mathbf{R}_j)_\delta O^{(l+1)}_{\alpha\beta\gamma(j)} + (\mathbf{R}_j)_\gamma O^{(l+1)}_{\alpha\beta\delta(j)} + (\mathbf{R}_j)_\beta O^{(l+1)}_{\alpha\gamma\delta(j)} + (\mathbf{R}_j)_\alpha O^{(l+1)}_{\beta\gamma\delta(j)}\right.\\
&\quad + (\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\delta Q^{(l+1)}_{\alpha\beta(j)} + (\mathbf{R}_j)_\beta(\mathbf{R}_j)_\delta Q^{(l+1)}_{\alpha\gamma(j)} + (\mathbf{R}_j)_\beta(\mathbf{R}_j)_\gamma Q^{(l+1)}_{\alpha\delta(j)}\\
&\quad + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\delta Q^{(l+1)}_{\beta\gamma(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\gamma Q^{(l+1)}_{\beta\delta(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\beta Q^{(l+1)}_{\gamma\delta(j)}\\
&\quad + (\mathbf{R}_j)_\beta(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\delta D^{(l+1)}_{\alpha(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\delta D^{(l+1)}_{\beta(j)}\\
&\quad + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\beta(\mathbf{R}_j)_\delta D^{(l+1)}_{\gamma(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\beta(\mathbf{R}_j)_\gamma D^{(l+1)}_{\delta(j)}\\
&\quad \left. + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\beta(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\delta M^{(l+1)}_{(j)}\right\}, \qquad (44)\\
T^{(l)}_{\alpha\beta\gamma\delta\epsilon} &= \sum_{j=1}^{8}\sum_i q_{i(j)}(\mathbf{a}_{i(j)}+\mathbf{R}_j)_\alpha(\mathbf{a}_{i(j)}+\mathbf{R}_j)_\beta(\mathbf{a}_{i(j)}+\mathbf{R}_j)_\gamma(\mathbf{a}_{i(j)}+\mathbf{R}_j)_\delta(\mathbf{a}_{i(j)}+\mathbf{R}_j)_\epsilon\\
&= \sum_{j=1}^{8}\left\{T^{(l+1)}_{\alpha\beta\gamma\delta\epsilon(j)} + (\mathbf{R}_j)_\epsilon H^{(l+1)}_{\alpha\beta\gamma\delta(j)} + (\mathbf{R}_j)_\delta H^{(l+1)}_{\alpha\beta\gamma\epsilon(j)}\right.\\
&\quad + (\mathbf{R}_j)_\gamma H^{(l+1)}_{\alpha\beta\delta\epsilon(j)} + (\mathbf{R}_j)_\beta H^{(l+1)}_{\alpha\gamma\delta\epsilon(j)} + (\mathbf{R}_j)_\alpha H^{(l+1)}_{\beta\gamma\delta\epsilon(j)}\\
&\quad + (\mathbf{R}_j)_\delta(\mathbf{R}_j)_\epsilon O^{(l+1)}_{\alpha\beta\gamma(j)} + (\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\epsilon O^{(l+1)}_{\alpha\beta\delta(j)} + (\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\delta O^{(l+1)}_{\alpha\beta\epsilon(j)}\\
&\quad + (\mathbf{R}_j)_\beta(\mathbf{R}_j)_\epsilon O^{(l+1)}_{\alpha\gamma\delta(j)} + (\mathbf{R}_j)_\beta(\mathbf{R}_j)_\delta O^{(l+1)}_{\alpha\gamma\epsilon(j)} + (\mathbf{R}_j)_\beta(\mathbf{R}_j)_\gamma O^{(l+1)}_{\alpha\delta\epsilon(j)}\\
&\quad + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\epsilon O^{(l+1)}_{\beta\gamma\delta(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\delta O^{(l+1)}_{\beta\gamma\epsilon(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\gamma O^{(l+1)}_{\beta\delta\epsilon(j)}\\
&\quad + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\beta O^{(l+1)}_{\gamma\delta\epsilon(j)}\\
&\quad + (\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\delta(\mathbf{R}_j)_\epsilon Q^{(l+1)}_{\alpha\beta(j)} + (\mathbf{R}_j)_\beta(\mathbf{R}_j)_\delta(\mathbf{R}_j)_\epsilon Q^{(l+1)}_{\alpha\gamma(j)} + (\mathbf{R}_j)_\beta(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\epsilon Q^{(l+1)}_{\alpha\delta(j)}\\
&\quad + (\mathbf{R}_j)_\beta(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\delta Q^{(l+1)}_{\alpha\epsilon(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\delta(\mathbf{R}_j)_\epsilon Q^{(l+1)}_{\beta\gamma(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\epsilon Q^{(l+1)}_{\beta\delta(j)}\\
&\quad + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\delta Q^{(l+1)}_{\beta\epsilon(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\beta(\mathbf{R}_j)_\epsilon Q^{(l+1)}_{\gamma\delta(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\beta(\mathbf{R}_j)_\delta Q^{(l+1)}_{\gamma\epsilon(j)}\\
&\quad + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\beta(\mathbf{R}_j)_\gamma Q^{(l+1)}_{\delta\epsilon(j)}\\
&\quad + (\mathbf{R}_j)_\beta(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\delta(\mathbf{R}_j)_\epsilon D^{(l+1)}_{\alpha(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\delta(\mathbf{R}_j)_\epsilon D^{(l+1)}_{\beta(j)}\\
&\quad + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\beta(\mathbf{R}_j)_\delta(\mathbf{R}_j)_\epsilon D^{(l+1)}_{\gamma(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\beta(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\epsilon D^{(l+1)}_{\delta(j)}\\
&\quad + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\beta(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\delta D^{(l+1)}_{\epsilon(j)}
\end{aligned}
$$

$$+(\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\beta(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\delta(\mathbf{R}_j)_\epsilon M^{(l+1)}_{(j)}\Big\}, \tag{45}$$

$$\begin{aligned}
U^{(l)}_{\alpha\beta\gamma\delta\epsilon\zeta} &= \sum_{j=1}^{8}\sum_{i} q_{i(j)}(\mathbf{a}_{i(j)}+\mathbf{R}_j)_\alpha(\mathbf{a}_{i(j)}+\mathbf{R}_j)_\beta(\mathbf{a}_{i(j)}+\mathbf{R}_j)_\gamma(\mathbf{a}_{i(j)}+\mathbf{R}_j)_\delta(\mathbf{a}_{i(j)}+\mathbf{R}_j)_\epsilon(\mathbf{a}_{i(j)}+\mathbf{R}_j)_\zeta \\
&= \sum_{j=1}^{8}\Big\{U^{(l+1)}_{\alpha\beta\gamma\delta\epsilon\zeta(j)} \\
&\quad + (\mathbf{R}_j)_\zeta T^{(l+1)}_{\alpha\beta\gamma\delta\epsilon(j)} + (\mathbf{R}_j)_\epsilon T^{(l+1)}_{\alpha\beta\gamma\delta\zeta(j)} + (\mathbf{R}_j)_\delta T^{(l+1)}_{\alpha\beta\gamma\epsilon\zeta(j)} \\
&\quad + (\mathbf{R}_j)_\gamma T^{(l+1)}_{\alpha\beta\delta\epsilon\zeta(j)} + (\mathbf{R}_j)_\beta T^{(l+1)}_{\alpha\gamma\delta\epsilon\zeta(j)} + (\mathbf{R}_j)_\alpha T^{(l+1)}_{\beta\gamma\delta\epsilon\zeta(j)} \\
&\quad + (\mathbf{R}_j)_\epsilon(\mathbf{R}_j)_\zeta H^{(l+1)}_{\alpha\beta\gamma\delta(j)} + (\mathbf{R}_j)_\delta(\mathbf{R}_j)_\zeta H^{(l+1)}_{\alpha\beta\gamma\epsilon(j)} + (\mathbf{R}_j)_\delta(\mathbf{R}_j)_\epsilon H^{(l+1)}_{\alpha\beta\gamma\zeta(j)} \\
&\quad + (\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\zeta H^{(l+1)}_{\alpha\beta\delta\epsilon(j)} + (\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\epsilon H^{(l+1)}_{\alpha\beta\delta\zeta(j)} + (\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\delta H^{(l+1)}_{\alpha\beta\epsilon\zeta(j)} \\
&\quad + (\mathbf{R}_j)_\beta(\mathbf{R}_j)_\zeta H^{(l+1)}_{\alpha\gamma\delta\epsilon(j)} + (\mathbf{R}_j)_\beta(\mathbf{R}_j)_\epsilon H^{(l+1)}_{\alpha\gamma\delta\zeta(j)} + (\mathbf{R}_j)_\beta(\mathbf{R}_j)_\delta H^{(l+1)}_{\alpha\gamma\epsilon\zeta(j)} \\
&\quad + (\mathbf{R}_j)_\beta(\mathbf{R}_j)_\gamma H^{(l+1)}_{\alpha\delta\epsilon\zeta(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\zeta H^{(l+1)}_{\beta\gamma\delta\epsilon(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\epsilon H^{(l+1)}_{\beta\gamma\delta\zeta(j)} \\
&\quad + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\delta H^{(l+1)}_{\beta\gamma\epsilon\zeta(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\gamma H^{(l+1)}_{\beta\delta\epsilon\zeta(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\beta H^{(l+1)}_{\gamma\delta\epsilon\zeta(j)} \\
&\quad + (\mathbf{R}_j)_\delta(\mathbf{R}_j)_\epsilon(\mathbf{R}_j)_\zeta O^{(l+1)}_{\alpha\beta\gamma(j)} + (\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\epsilon(\mathbf{R}_j)_\zeta O^{(l+1)}_{\alpha\beta\delta(j)} + (\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\delta(\mathbf{R}_j)_\zeta O^{(l+1)}_{\alpha\beta\epsilon(j)} \\
&\quad + (\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\delta(\mathbf{R}_j)_\epsilon O^{(l+1)}_{\alpha\beta\zeta(j)} + (\mathbf{R}_j)_\beta(\mathbf{R}_j)_\epsilon(\mathbf{R}_j)_\zeta O^{(l+1)}_{\alpha\gamma\delta(j)} + (\mathbf{R}_j)_\beta(\mathbf{R}_j)_\delta(\mathbf{R}_j)_\zeta O^{(l+1)}_{\alpha\gamma\epsilon(j)} \\
&\quad + (\mathbf{R}_j)_\beta(\mathbf{R}_j)_\delta(\mathbf{R}_j)_\epsilon O^{(l+1)}_{\alpha\gamma\zeta(j)} + (\mathbf{R}_j)_\beta(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\zeta O^{(l+1)}_{\alpha\delta\epsilon(j)} + (\mathbf{R}_j)_\beta(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\epsilon O^{(l+1)}_{\alpha\delta\zeta(j)} \\
&\quad + (\mathbf{R}_j)_\beta(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\delta O^{(l+1)}_{\alpha\epsilon\zeta(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\epsilon(\mathbf{R}_j)_\zeta O^{(l+1)}_{\beta\gamma\delta(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\delta(\mathbf{R}_j)_\zeta O^{(l+1)}_{\beta\gamma\epsilon(j)} \\
&\quad + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\delta(\mathbf{R}_j)_\epsilon O^{(l+1)}_{\beta\gamma\zeta(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\zeta O^{(l+1)}_{\beta\delta\epsilon(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\epsilon O^{(l+1)}_{\beta\delta\zeta(j)} \\
&\quad + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\delta O^{(l+1)}_{\beta\epsilon\zeta(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\beta(\mathbf{R}_j)_\zeta O^{(l+1)}_{\gamma\delta\epsilon(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\beta(\mathbf{R}_j)_\epsilon O^{(l+1)}_{\gamma\delta\zeta(j)} \\
&\quad + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\beta(\mathbf{R}_j)_\delta O^{(l+1)}_{\gamma\epsilon\zeta(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\beta(\mathbf{R}_j)_\gamma O^{(l+1)}_{\delta\epsilon\zeta(j)} \\
&\quad + (\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\delta(\mathbf{R}_j)_\epsilon(\mathbf{R}_j)_\zeta Q^{(l+1)}_{\alpha\beta(j)} + (\mathbf{R}_j)_\beta(\mathbf{R}_j)_\delta(\mathbf{R}_j)_\epsilon(\mathbf{R}_j)_\zeta Q^{(l+1)}_{\alpha\gamma(j)} \\
&\quad + (\mathbf{R}_j)_\beta(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\epsilon(\mathbf{R}_j)_\zeta Q^{(l+1)}_{\alpha\delta(j)} + (\mathbf{R}_j)_\beta(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\delta(\mathbf{R}_j)_\zeta Q^{(l+1)}_{\alpha\epsilon(j)} \\
&\quad + (\mathbf{R}_j)_\beta(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\delta(\mathbf{R}_j)_\epsilon Q^{(l+1)}_{\alpha\zeta(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\delta(\mathbf{R}_j)_\epsilon(\mathbf{R}_j)_\zeta Q^{(l+1)}_{\beta\gamma(j)} \\
&\quad + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\epsilon(\mathbf{R}_j)_\zeta Q^{(l+1)}_{\beta\delta(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\delta(\mathbf{R}_j)_\zeta Q^{(l+1)}_{\beta\epsilon(j)} \\
&\quad + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\delta(\mathbf{R}_j)_\epsilon Q^{(l+1)}_{\beta\zeta(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\beta(\mathbf{R}_j)_\epsilon(\mathbf{R}_j)_\zeta Q^{(l+1)}_{\gamma\delta(j)} \\
&\quad + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\beta(\mathbf{R}_j)_\delta(\mathbf{R}_j)_\zeta Q^{(l+1)}_{\gamma\epsilon(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\beta(\mathbf{R}_j)_\delta(\mathbf{R}_j)_\epsilon Q^{(l+1)}_{\gamma\zeta(j)} \\
&\quad + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\beta(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\zeta Q^{(l+1)}_{\delta\epsilon(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\beta(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\epsilon Q^{(l+1)}_{\delta\zeta(j)} \\
&\quad + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\beta(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\delta Q^{(l+1)}_{\epsilon\zeta(j)} \\
&\quad + (\mathbf{R}_j)_\beta(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\delta(\mathbf{R}_j)_\epsilon(\mathbf{R}_j)_\zeta D^{(l+1)}_{\alpha(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\delta(\mathbf{R}_j)_\epsilon(\mathbf{R}_j)_\zeta D^{(l+1)}_{\beta(j)} \\
&\quad + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\beta(\mathbf{R}_j)_\delta(\mathbf{R}_j)_\epsilon(\mathbf{R}_j)_\zeta D^{(l+1)}_{\gamma(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\beta(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\epsilon(\mathbf{R}_j)_\zeta D^{(l+1)}_{\delta(j)} \\
&\quad + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\beta(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\delta(\mathbf{R}_j)_\zeta D^{(l+1)}_{\epsilon(j)} + (\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\beta(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\delta(\mathbf{R}_j)_\epsilon D^{(l+1)}_{\zeta(j)} \\
&\quad +(\mathbf{R}_j)_\alpha(\mathbf{R}_j)_\beta(\mathbf{R}_j)_\gamma(\mathbf{R}_j)_\delta(\mathbf{R}_j)_\epsilon(\mathbf{R}_j)_\zeta M^{(l+1)}_{(j)}\Big\}.
\end{aligned} \tag{46}$$

2.2.2 Origin Shift in Downward Path

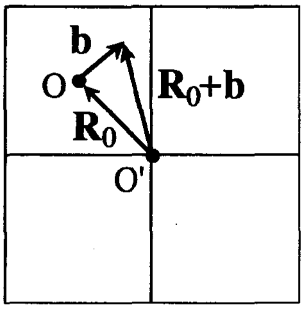


Figure 7: A schematic diagram showing the origin shift in the downward pass. The symbol O is the origin (center) of the current box at level l and O' is the origin of its parent box at level $l-1$.

The coefficients of the Taylor expansion, $\{\Psi^{(l)}, \Psi^{(l)}_\alpha, \ldots\}$, can be obtained from those of parent box, $\{\Psi^{(l-1)}, \Psi^{(l-1)}_\alpha, \ldots\}$, by shifting the origin from parent box to the current box at level l (Fig. 7).

$$\begin{aligned}
\Phi^{(l)}_{outside} &= \Phi^{(l-1)} \text{ with shifted origin} \\
&= \Psi^{(l-1)} + \sum_\alpha \Psi^{(l-1)}_\alpha (\mathbf{R_0}+\mathbf{b})_\alpha + \sum_{\alpha\beta} \Psi^{(l-1)}_{\alpha\beta} (\mathbf{R_0}+\mathbf{b})_\alpha (\mathbf{R_0}+\mathbf{b})_\beta \\
&\quad + \sum_{\alpha\beta\gamma} \Psi^{(l-1)}_{\alpha\beta\gamma} (\mathbf{R_0}+\mathbf{b})_\alpha (\mathbf{R_0}+\mathbf{b})_\beta (\mathbf{R_0}+\mathbf{b})_\gamma \\
&\quad + \sum_{\alpha\beta\gamma\delta} \Psi^{(l-1)}_{\alpha\beta\gamma\delta} (\mathbf{R_0}+\mathbf{b})_\alpha (\mathbf{R_0}+\mathbf{b})_\beta (\mathbf{R_0}+\mathbf{b})_\gamma (\mathbf{R_0}+\mathbf{b})_\delta \\
&\quad + \sum_{\alpha\beta\gamma\delta\epsilon} \Psi^{(l-1)}_{\alpha\beta\gamma\delta\epsilon} (\mathbf{R_0}+\mathbf{b})_\alpha (\mathbf{R_0}+\mathbf{b})_\beta (\mathbf{R_0}+\mathbf{b})_\gamma (\mathbf{R_0}+\mathbf{b})_\delta (\mathbf{R_0}+\mathbf{b})_\epsilon \\
&\quad + \sum_{\alpha\beta\gamma\delta\epsilon\zeta} \Psi^{(l-1)}_{\alpha\beta\gamma\delta\epsilon\zeta} (\mathbf{R_0}+\mathbf{b})_\alpha (\mathbf{R_0}+\mathbf{b})_\beta (\mathbf{R_0}+\mathbf{b})_\gamma (\mathbf{R_0}+\mathbf{b})_\delta (\mathbf{R_0}+\mathbf{b})_\epsilon (\mathbf{R_0}+\mathbf{b})_\zeta \\
&= \Psi^{(l)} + \sum_\alpha \Psi^{(l)}_\alpha (\mathbf{b})_\alpha + \sum_{\alpha\beta} \Psi^{(l)}_{\alpha\beta} (\mathbf{b})_\alpha (\mathbf{b})_\beta + \sum_{\alpha\beta\gamma} \Psi^{(l)}_{\alpha\beta\gamma} (\mathbf{b})_\alpha (\mathbf{b})_\beta (\mathbf{b})_\gamma \\
&\quad + \sum_{\alpha\beta\gamma\delta} \Psi^{(l)}_{\alpha\beta\gamma\delta} (\mathbf{b})_\alpha (\mathbf{b})_\beta (\mathbf{b})_\gamma (\mathbf{b})_\delta + \sum_{\alpha\beta\gamma\delta\epsilon} \Psi^{(l)}_{\alpha\beta\gamma\delta\epsilon} (\mathbf{b})_\alpha (\mathbf{b})_\beta (\mathbf{b})_\gamma (\mathbf{b})_\delta (\mathbf{b})_\epsilon \\
&\quad + \sum_{\alpha\beta\gamma\delta\epsilon\zeta} \Psi^{(l)}_{\alpha\beta\gamma\delta\epsilon\zeta} (\mathbf{b})_\alpha (\mathbf{b})_\beta (\mathbf{b})_\gamma (\mathbf{b})_\delta (\mathbf{b})_\epsilon (\mathbf{b})_\zeta,
\end{aligned} \tag{47}$$

where

$$\begin{aligned}
\Psi^{(l)} &= \Psi^{(l-1)} + \sum_\alpha (\mathbf{R_0})_\alpha \Psi^{(l-1)}_\alpha + \sum_{\alpha\beta} (\mathbf{R_0})_\alpha (\mathbf{R_0})_\beta \Psi^{(l-1)}_{\alpha\beta} \\
&\quad + \sum_{\alpha\beta\gamma} (\mathbf{R_0})_\alpha (\mathbf{R_0})_\beta (\mathbf{R_0})_\gamma \Psi^{(l-1)}_{\alpha\beta\gamma} + \sum_{\alpha\beta\gamma\delta} (\mathbf{R_0})_\alpha (\mathbf{R_0})_\beta (\mathbf{R_0})_\gamma (\mathbf{R_0})_\delta \Psi^{(l-1)}_{\alpha\beta\gamma\delta} \\
&\quad + \sum_{\alpha\beta\gamma\delta\epsilon} (\mathbf{R_0})_\alpha (\mathbf{R_0})_\beta (\mathbf{R_0})_\gamma (\mathbf{R_0})_\delta (\mathbf{R_0})_\epsilon \Psi^{(l-1)}_{\alpha\beta\gamma\delta\epsilon} \\
&\quad + \sum_{\alpha\beta\gamma\delta\epsilon\zeta} (\mathbf{R_0})_\alpha (\mathbf{R_0})_\beta (\mathbf{R_0})_\gamma (\mathbf{R_0})_\delta (\mathbf{R_0})_\epsilon (\mathbf{R_0})_\zeta \Psi^{(l-1)}_{\alpha\beta\gamma\delta\epsilon\zeta},
\end{aligned} \tag{48}$$

$$\begin{aligned}
\Psi_{\alpha}^{(l)} &= \Psi_{\alpha}^{(l-1)} + 2\sum_{\beta}(\mathbf{R}_0)_\beta \Psi_{\alpha\beta}^{(l-1)} + 3\sum_{\beta\gamma}(\mathbf{R}_0)_\beta(\mathbf{R}_0)_\gamma \Psi_{\alpha\beta\gamma}^{(l-1)} \\
&+ 4\sum_{\beta\gamma\delta}(\mathbf{R}_0)_\beta(\mathbf{R}_0)_\gamma(\mathbf{R}_0)_\delta \Psi_{\alpha\beta\gamma\delta}^{(l-1)} + 5\sum_{\beta\gamma\delta\epsilon}(\mathbf{R}_0)_\beta(\mathbf{R}_0)_\gamma(\mathbf{R}_0)_\delta(\mathbf{R}_0)_\epsilon \Psi_{\alpha\beta\gamma\delta\epsilon}^{(l-1)} \\
&+ 6\sum_{\beta\gamma\delta\epsilon\zeta}(\mathbf{R}_0)_\beta(\mathbf{R}_0)_\gamma(\mathbf{R}_0)_\delta(\mathbf{R}_0)_\epsilon(\mathbf{R}_0)_\zeta \Psi_{\alpha\beta\gamma\delta\epsilon\zeta}^{(l-1)}, \qquad (49)
\end{aligned}$$

$$\begin{aligned}
\Psi_{\alpha\beta}^{(l)} &= \Psi_{\alpha\beta}^{(l-1)} + 3\sum_{\gamma}(\mathbf{R}_0)_\gamma \Psi_{\alpha\beta\gamma}^{(l-1)} + 6\sum_{\gamma\delta}(\mathbf{R}_0)_\gamma(\mathbf{R}_0)_\delta \Psi_{\alpha\beta\gamma\delta}^{(l-1)} \\
&+ 10\sum_{\gamma\delta\epsilon}(\mathbf{R}_0)_\gamma(\mathbf{R}_0)_\delta(\mathbf{R}_0)_\epsilon \Psi_{\alpha\beta\gamma\delta\epsilon}^{(l-1)} \\
&+ 15\sum_{\gamma\delta\epsilon\zeta}(\mathbf{R}_0)_\gamma(\mathbf{R}_0)_\delta(\mathbf{R}_0)_\epsilon(\mathbf{R}_0)_\zeta \Psi_{\alpha\beta\gamma\delta\epsilon\zeta}^{(l-1)}, \qquad (50)
\end{aligned}$$

$$\begin{aligned}
\Psi_{\alpha\beta\gamma}^{(l)} &= \Psi_{\alpha\beta\gamma}^{(l-1)} + 4\sum_{\delta}(\mathbf{R}_0)_\delta \Psi_{\alpha\beta\gamma\delta}^{(l-1)} + 10\sum_{\delta\epsilon}(\mathbf{R}_0)_\delta(\mathbf{R}_0)_\epsilon \Psi_{\alpha\beta\gamma\delta\epsilon}^{(l-1)} \\
&+ 20\sum_{\delta\epsilon\zeta}(\mathbf{R}_0)_\delta(\mathbf{R}_0)_\epsilon(\mathbf{R}_0)_\zeta \Psi_{\alpha\beta\gamma\delta\epsilon\zeta}^{(l-1)}, \qquad (51)
\end{aligned}$$

$$\Psi_{\alpha\beta\gamma\delta}^{(l)} = \Psi_{\alpha\beta\gamma\delta}^{(l-1)} + 5\sum_{\epsilon}(\mathbf{R}_0)_\epsilon \Psi_{\alpha\beta\gamma\delta\epsilon}^{(l-1)} + 15\sum_{\epsilon\zeta}(\mathbf{R}_0)_\epsilon(\mathbf{R}_0)_\zeta \Psi_{\alpha\beta\gamma\delta\epsilon\zeta}^{(l-1)}, \qquad (52)$$

$$\Psi_{\alpha\beta\gamma\delta\epsilon}^{(l)} = \Psi_{\alpha\beta\gamma\delta\epsilon}^{(l-1)} + 6\sum_{\zeta}(\mathbf{R}_0)_\zeta \Psi_{\alpha\beta\gamma\delta\epsilon\zeta}^{(l-1)}, \qquad (53)$$

$$\Psi_{\alpha\beta\gamma\delta\epsilon\zeta}^{(l)} = \Psi_{\alpha\beta\gamma\delta\epsilon\zeta}^{(l-1)}. \qquad (54)$$

3 Model Calculations

This section describes model calculations using our implementations of the FMM. The errors and timings as functions of system size (N), the screening parameter (κ) and the FMM parameters (p, ws, l) are investigated. Our model system is the spherically confined charged particles, interacting mutually via the Yukawa potential. The charges are randomly distributed inside a sphere of radius 0.5 within a $1\times1\times1$ box. In our case, the magnitudes and signs of each particle's charge are chosen equally to be q, while most systems reported for Coulomb interacting system ($\kappa = 0$) have been charge-neutral, which is likely to underestimate the errors of the FMM calculations.

3.1 Timings

In Fig. 8, we show the FMM timings with $ws = 1$ and $ws = 2$ as a function of system size. The order of expansions, p, is fixed at 6. The level of subdivision is changed so as to minimize the timings for each ws. All timings are from calculations run on a PC (Pentium III 600 MHz machine with 512 MB of RAM). We observe that timings increase quadratically for fixed level of subdivisions. As described in the previous section, the interactions between the particles in the nearest neighbor boxes are calculated directly, which contribute to the quadratic behavior of timings since the number of pairs of particles increases quadratically with respect to the number of particles in the nearest neighbor boxes. For small system size, the timings have constant values, though the results are not plotted in Fig. 8. The computational cost of the upward and downward pass is independent of the system size and depends only on the FMM parameters (l, p, ws). This constant values increase with the increase of ws. For larger ws, we have much larger number of boxes in the interaction list. There are 189 boxes for $ws = 1$ and 875 for $ws = 2$. With the number of particles in the smallest box constant, the timings increase almost linearly with respect to system size N, as we expected.

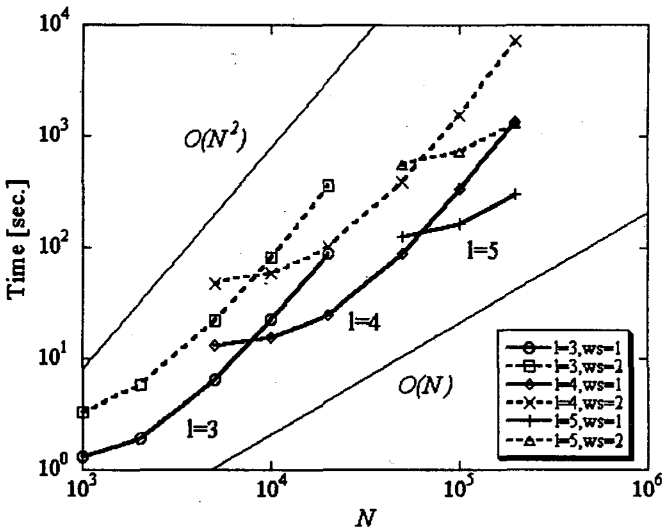


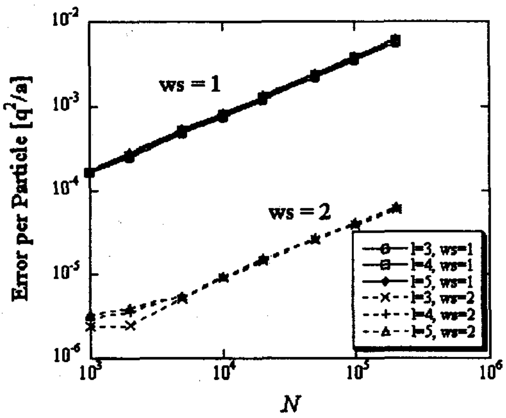
Figure 8: CPU time required for one MD step as a function of the number of particles N. The thick solid and broken lines represent the results for $ws = 1$ and $ws = 2$, respectively.

3.2 Errors

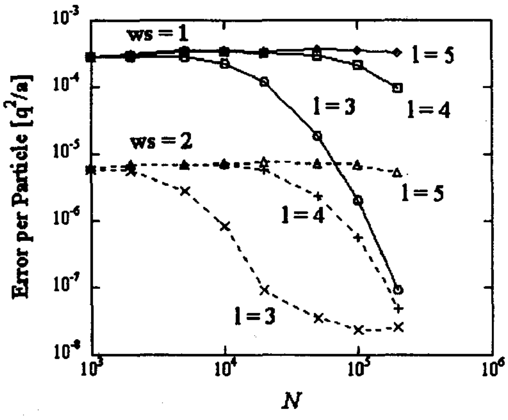
The interaction energies per particle in units of q^2/a are calculated. The deviation between these energies and the exact results obtained by calculating directly all pairs of interactions is reported as our error. In Fig. 9, the FMM errors with $ws = 1$ and $ws = 2$ are plotted as a function of the system size. The value of p is fixed at 6. ξ is the parameter specifying the strength of screening defined by $\xi = \kappa a$, where a is the mean distance between particles. For $\xi > 1$, the error decreases with the system size for fixed level of subdivisions. The maximum value of error decreases with increase in ξ. However, for Coulomb system ($\xi = 0$), the error increases with the system size. This indicates that we need a special care for large systems with pure Coulomb interaction.

4 Conclusion

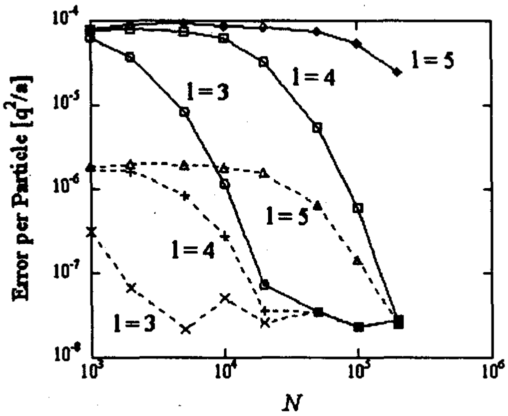
We have described mathematical expressions of the FMM which are necessary for a large-scale molecular dynamics of the Yukawa system. Model simulations have also been performed to test our implementation and its efficiency of the FMM. It is shown that the computational complexity scales linearly with respect to system size.



(a) $\xi = 0.0$



(b) $\xi = 1.0$



(c) $\xi = 2.0$

Figure 9: The errors in the interaction energy per particle as a function of the number of particles N in the system with (a) $\xi = 0.0$, (b) $\xi = 1.0$, and (c) $\xi = 2.0$. The solid and broken lines represent the results for $ws = 1$ and $ws = 2$, respectively.

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