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An improved FMM Algorithm of the 3D-linearized Poisson-Boltzmann equation

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Abstract: This paper presents a new FMM algorithm for the linearized Poisson-Boltzmann equation in three dimensions. The performance of the proposed algorithm is assessed on a example in three dimensions and compared with the direct method. The numerical results show the power of the new method, that allow to achieve the best schemes to reduce the time of the particle interactions, which are based on diagonal form of translation operators for linearized Poisson-Boltzmann equation.

Keywords: The linearized Poisson-Boltzmann equation; Translation operators; Fast multipole method algorithm.

1 Introduction

The solution of integral equation by elementary boundary integral methods usually leads to solve systems of linear equations, whose matrix is complex, full and non-symmetric. This type of problem has been extensively studied and we can identify two main methods of resolution.

The first is the direct schemes, which factorize the matrix. The second method is the iterative schemes which require the application of the matrix of the system to a sequence of recursively generated vectors. For the first method, once the matrix is factorized one can solve the system for second additional members at a reduced cost compared to the factorization.

One of the standard approaches based on the factorization is LU (nonsymmetric matrix) or L^TUL (symmetric matrix). On the other side, when the matrixes are generated by the boundary element method, which are full, and when the number of unknown nodal becomes high, the direct schemes are very expensive in computing time and memory space. For a system with N degrees of freedom, the storage of the matrix is of the order of $O(N^2)$, and the solution time grows to $O(N^3)$. On current personal computers, these conditions limit us for a problem whose size is of the order of tens of thousands of unknown nodals, and that limits the possible applications. For this reason in practice iterative methods are attractive. The storage of the matrix is no longer necessary and the process is accelerated. Each iteration typically uses a matrix-vector product which leads to computation time of order $O(nN^2)$, where n is much lower than the number of unknown systems. The solution ends when the residual is less than a limit set in advance by the user. To do this each iteration has a specific strategy but they are all based on the same principle. On the same subject, for example there are many recent works about the fixed point theorems [48,49].

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The main step of the iterative methods is evaluation at each iteration, of the residual :

$$B - AU$$

which needs to carry out the product of the test vector U by the matix A. In the general case where the matrix is full, the computation time is of order $O(nN^2)$ operations. Moreover, it is now well known, that this computational cost may be drastically reduced for the systems issued from the interaction problems, using the so called the Fast Multipole Methods (FMM), which was originally introduced by Rokhlin and Greengard [1] for the simulation of systems with large numbers of interacting particles.

The advantages of the FMM can be huge when large numbers of particles are involved, as it reduces the complexity of calculations from $O(N^2)$ to $O(N)$. The cost of a matrix-vector product becomes an order $O(N)$ for solving static problems (Laplace's equation or elastostatic) and an order $O(N\log(N))$ for dynamic problems (Helmholtz, Maxwell).

The FMM was then extended to investigate the N-body problems such as the Lennard-Jones Potential [3]. An FMM for the Helmholtz equation in $2D$ was published in the article [8] then in $3D$ [9]. These algorithms lead to complexity of $O(N^{3/2})$ for the single-level FMM, which have been improved by R.L. Wagner and W.C. Chew [10] using the concept of propagation of rays. The multi-level version has been developed in two dimensions in [11], and in three dimensions in [12] by the team of W.C. Chew. E. Darve presented the multi-level FMM for the Helmholtz/Maxwell equations [13,14]. Through the work of Rokhlin for the Helmholtz equation [15,16,17], he leads to algorithms of order $O(N\log N)$. For specific details on the error estimates, we refer the reader to the article of E. Darve [18]. Similarly, for a numerical study of the method, we refer to the article [19]. Given the interest of this method, many applications are being considered such as an FMM for the Maxwell equation which was published in [20,**?**], or the inverse problems [22]. They have also been applied in other fields of application in numerical analysis such as molecular dynamics [23] or multidimensional integrals [24] and in many other domains such as the problems of linear elasticity [25] or establishing a fast Gauss transform [26]. Since, it conquers all fields of physics, It is especially used in electromagnetism [27,28] and now appears in mechanics [29,30]. As part of the multipole method, many recent research such as the Fast Multipole accelerated BEM for $3D$ visco-elastodynamic [31,32] was developped.

The FMM was introduced in the early eighties to solve problems of electrostatic with $O(N)$ charges and $O(N)$ observation points. The idea of the method introduced by Rokhlin and Greengard is to accelerate the calculation by making calculations with ≪packages≫. More precisely, the FMM can be used to reduce the number of operations performed by two ideas. The first will be to create the ≪packages≫ of sources, i.e. an equivalent source which represents the sources at distances more than its own length away from observations points. The second idea is to create an observation point which represents the group sufficiently far from the ≪packages≫ of point sources considered. The question then is the know how will be constructed these ≪packages≫? The idea, which was adopted by all multipole algorithms is to divide the domain into cubic boxes (in the three-dimensional case). In practice, this is translated by two important things. The first is an addition formula, which is related to the physics of the problem and which expresses the effect of a distant point source as sum of multipole contributions. The second is the algorithm, which is the heart of the method.

More specifically, we describe here an algorithm for the rapid evaluation of expressions of the form

$$\Phi_i = \sum_{j=1, j\neq i}^{N} w_j G(x_j - x_i) \tag{1}$$

where Φ_i is the potential due to the point x_i and G is a Green's function, given $x_1,...,x_N \in \mathbb{R}^3$ and $w_1,...,w_N \in \mathbb{R}^3$.

The algorithm of the FMM construct a hierarchical subdivision of the domain into cubic boxes, in which it is recursively divided into smaller and smaller boxes. For each region in the hierarchy, the ≪far-field expansion≫ is used. In fact, the data structure is equivalent to the notion of recursive function of tree. It will be naturally used here. A tree consists of a single node or a node and a set of subtrees. If a branch connects a node n_i to a node n_j located a floor below, we say that n_i is the father of n_j (and n_j the child of n_i). The only node with no parent is the root of the tree. All nodes having no son are called leaf. The level of a node is its generation from the root (the root is the level 0, its childs are the level 1,...). Each node will be for us associated to a box. So there will be a correspondence between the abstract structure of the tree and the division of the domain into boxes.

Now how to build the tree? To start with, we take the smallest cubical box which encloses all the points x_i, this box is the root of the tree. and then constructs a hierarchical subdivision of that box, in which it is divided into eight boxes of equal size, each of these boxes were a son of the root. Then repeat the subdivision process recursively until for example, the lowest-level boxes (the leaf) has a maximum preselected number points in them. Note that at a given level all boxes have the same size. In the literature this type of tree is called *oct-tree*, indeed, each box has a maximum number of child equal to eight. At each level, we kept in the tree that nonblank boxes (ie boxes have one points at least). A ≪far-field expansion≫ is produced for each box, which represents the potential due to the points on that box, at distances more than its own length away from it. The ≪far-field expansion≫ for each "childless" box is calculated from the points on that box; the ≪far-field expansion≫ for each father box is calculated from the ≪far-field expansion≫ of its children. These ≪far-field expansion≫ are not evaluated directly but translated into ≪local expansions≫, which represent the potential inside a box due to points distant from that box. ≪local expansions≫ on father boxes are evaluated by translating them into ≪local expansions≫ on their children; then the ≪local expansions≫ on each childless box is evaluated on the points x_i in that box.

The Algorithm of the FMM uses the addition formula as efficiently as possible. We can imagine that the addition formula is a development in a Taylor series around a point of the fundamental solution, this is sometimes the case. Now, we present an abstract generic addition formula, which is a representation of what is treated in each problem.

The addition formula is a series expansion of the Green's function around an origin point x_0 arbitrarily selected, that we can present under the generic form:

$$G(y-x) = G(r+r_0) = \sum_n \sum_{m=-n}^{n} I_n^m(r_0) J_n^m(r) \ \text{ in } \ 3D \tag{2}$$

and under the generic form

$$G(y-x) = G(r+r_0) = \sum_n I_n(r_0) J_n(r) \ \text{ in } \ 2D \tag{3}$$

where $r = |y-x_0|$ and $r_0 = |x_0-x|$, the formulas (2),(3) are valid under certain conditions, a typical condition is $|r| > |r_0|$. The factors I_n^m, J_n^m, I_n and J_n are known analytically and dependent of the fundamental solution used.

For numerical calculations, in order to use the algorithm of the FMM, in general case the Green function must satisfy the flowing condition and the series must be truncated to a number p of terms.

$$G(y-x) = G(r+r_0) = \sum_{n=0}^{p} I_n(r_0) J_n(r) + \varepsilon(p, \frac{|\,r\,|}{|\,r_0\,|}) \tag{4}$$

where $\varepsilon(p, \frac{|r|}{|r_0|})$ is a decreasing function on $\frac{|r|}{|r_0|}$ and p.

The addition formula (3) is accompanied by the formulas of changing of origin, which are on the form:

$$J_n(y-x) = \sum_{n'} I_{n'}(r_0) J_{n+n'}(r) \tag{5}$$

$$I_n(y-x) = \sum_{n'} I_{n'}(r_0) I_{n-n'}(r) \tag{6}$$

In generally case, these formulas appeared as a discrete convolution for three-dimensional case. We note that using the formulas (5) and (6) allows us to symmetrize the addition formula, by using a series expansion around two points x_0 and y_0.

$$\begin{aligned} G(y-x) &= G(y-y_0+y_0-x_0+x_0-x) \\ &= \sum_{n} I_n(x_0-x) J_n(y-y_0+y_0-x_0) \\ &= \sum_{n,n'} I_n(x_0-x) J_{n+n'}(y_0-x_0) I_{n'}(y-y_0) \end{aligned} \tag{7}$$

These formulas are used to create the ≪far-field expansion≫ and the ≪local expansions≫.

In this paper, we introduce some new technique such as rotation, plane wave representation and an improved algorithm to accelerate the matrix-vector multiplication of the Yukawa potential, that accur in particle physics. The Yukawa potential defined by:

$$V(r) = \frac{e^{-\lambda r}}{r} \tag{8}$$

where λ is a real constant and r is the radial distance to the particle.

Let's consider a set of particles with locations $x_1, x_2, ..., x_N$ in three-dimensional space and $q_1, q_2, ..., q_N$ the corresponding charge strengths, the potential at $x_i, i = 1...N$ due to all the other particles is:

$$\Phi(x_j) = \sum_{i=1, i\neq j}^{N} q_i \frac{e^{-\lambda \|x_j - x_i\|}}{\|x_j - x_i\|} \text{ avec } \lambda \in \mathbb{R}^3 \tag{9}$$

where $\lambda \in \mathbb{R}$.

The Yukawa potential is considered an important issue since it was used in many areas of sciences as: physics, high energy physics [33,34], chemistry and biology. This potential is the Green function of the partial differential equation:

$$\nabla^2 \Phi - \lambda^2 \Phi = f(x) \tag{10}$$

The Yukawa potential, which occurs in implicit marching schemes for the parabolic equations, in Debye-Huckel theory [35] and Navier-Stokes equations. It can also be viewed as the linearized Poisson-Boltzmann equation in biochemistry and biophysics [36,37]. In the next section, we provide the necessary formulae of the method.

2 Mathematical preliminaries

In this section, we describe the operators $T_{PM}, T_{MM}, T_{ML}, T_{LL}, T_{LP}$ needed by the algorithme of the new version of the FMM in order to accelrate the matrix-vector product (9). For further details see [39].

The modified spherical Hankel and modified spherical Bessel functions $k_n(r)$, $i_n(r)$ are defined in terms of the Bessel function $\mathscr{J}_n(z)$ by

$$I_\nu(r) = i^{-\nu}\mathscr{J}_\nu(ir) \ \ (i=\sqrt{-1}),$$
$$K_\nu(r) = \frac{\pi}{2\sin(\nu\pi)}\left(I_{-\nu}(r) - I_\nu(r)\right)$$
$$k_n(r) = \sqrt{\frac{\pi}{2r}}K_{n+\frac{1}{2}}(r)$$
$$i_n(r) = \sqrt{\frac{\pi}{2r}}I_{n+\frac{1}{2}}(r)$$

and let P_n denote the Legendre polynomial an nth-degree. Each spherical harmonics Y_n^m is a nth-degree and order m. That can be defined by the formula:

$$Y_n^m(\theta,\varphi) = \sqrt{\frac{(2n+1)}{4\pi}\frac{(n-m)!}{(n+m)!}}.P_n^{|m|}(\cos(\theta))e^{im\varphi} \tag{11}$$

where the associated Legendre function is P_n^m, It may be expressed using Rodrigues' formula

$$P_n^m(x) = \frac{(-1)^m}{2^n n!}(1-x^2)^{\frac{m}{2}}\frac{d^{n+m}}{dx^{n+m}}(x^2-1)^n \ \forall (n,m) \in IN^2 \text{ avec } 0 \le m \le n.$$

In particular,

$$k_0(\lambda r) = \frac{\pi}{2}\frac{e^{-\lambda r}}{\lambda r}.$$

Using these special functions and the the Grafś addition theorem [39] we can produce the far field induced by a collection of point sources.

Theorem 2.1.(Operator T_{PM}). Suppose that N strengths $(q_i)_{i\in[|1,N|]}$ are located at points $x_{i\in[|1,N|]}$ with spherical coordinates $(\rho_i,\alpha_i,\beta_i)_{i\in[|1,N|]}$, respectively. Suppose further that the points $x_{i\in[|1,N|]}$ are inside a sphere of radius a centered at the origin. Then for any point $x=(r,\theta,\phi)\in\mathbb{R}^3\backslash D$, the potential $\Phi(x)$ generated by the strengths $(q_i)_{i\in[|1,N|]}$ is equal to:

$$\Phi(x) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} M_n^m k_n(\lambda r)Y_n^m(\theta,\phi)$$

where

$$M_n^m = 8\lambda\sum_{i=1}^{N} q_i.i_n(\lambda\rho_i).Y_n^{-m}(\alpha_i,\beta_i) \ \forall (n,m)\in\mathbb{N}\times\mathbb{Z} \text{ avec } 0\le|\ m\ |\le n. \tag{12}$$

Theorem 2.2. (Operator T_{MM}) Suppose that N strengths $(q_i)_{i\in[|1,N|]}$ are located at points $x_{i\in[|1,N|]}$ with spherical coordinates $(\rho_i,\alpha_i,\beta_i)_{i\in[|1,N|]}$, respectively. Suppose that the points $x_{i\in[|1,N|]}$ are inside the sphere D of radius a centered at $x_0=(\rho,\alpha,\beta)$. Then for any point $x=(r,\theta,\phi)\in\mathbb{R}^3\backslash D$, the potential $\Phi(x)$ generated by the strengths $(q_i)_{i\in[|1,N|]}$ is

described by the multipole expansion:

$$\Phi(x) = \sum_{j=0}^{\infty} \sum_{k=-j}^{j} M_j^k k_j(\lambda r^{'}) Y_j^k(\theta^{'}, \phi^{'}) \tag{13}$$

$(\rho^{'}, \alpha^{'}, \beta^{'})$ are the spherical coordinates of the vector $x - x_0$.

Suppose that D_1 is the sphere centered at the origin and of radius $(a_1 = a + \rho)$. Then, for any point $x = (r, \theta, \phi) \in \mathbb{R}^3 \backslash D_1$ the field can be described by

$$\Phi(x) = \sum_{j=0}^{\infty} \sum_{k=-j}^{j} O_j^k k_j(\lambda r) Y_j^k(\theta, \phi). \tag{14}$$

Definition 2.3. We denote by T_{MM}, the diagonal operator maping the harmonic expansion M_n^m to the shift harmonic expansion O_n^m.

Theorem 2.4. (Operator T_{ML}) Suppose that N strengths $(q_i)_{i\in[|1,N|]}$ are located at points $x_{i\in[|1,N|]}$ with spherical coordinates $(\rho_i, \alpha_i, \beta_i)_{i\in[|1,N|]}$ are inside the sphere D of radius a centered at $x_0 = (\rho, \alpha, \beta)$, and that $\rho > (c+1)a$ for some $c > 1$. Then for any point $x = (r, \theta, \phi) \in D$, the potential $\Phi(x)$ is given by a local expansion

$$\Phi(x) = \sum_{j=0}^{\infty} \sum_{k=-j}^{j} L_j^k i_j(\lambda r) Y_j^k(\theta, \phi). \tag{15}$$

Definition 2.5. We denote by T_{ML} the linear operator maping the coefficients in a harmonic expansion M_n^m to the coefficient in the corresponding harmonic expansion L_n^m.

Theorem 2.6. (Operator T_{LL}) Suppose that N strengths $(q_i)_{i\in[|1,N|]}$ are located at points $x_{i\in[|1,N|]}$ with spherical coordinates $(\rho_i, \alpha_i, \beta_i)_{i\in[|1,N|]}$ are inside a sphere D of radius a centered at the origin. Suppose further that for any point $x = (r, \theta, \phi) \in D$, the potential $\Phi(x)$ can be described by the local expansion

$$\Phi(x) = \sum_{j=0}^{p} \sum_{k=-j}^{j} L_j^k i_j(\lambda r) Y_j^k(\theta, \phi) \tag{16}$$

Let $x_0 = (\rho, \alpha, \beta) \in D$ then the field in the neighborhood of x_0 can be described by a local expansion

$$\Phi(x) = \sum_{j=0}^{\infty} \sum_{k=-j}^{j} W_j^k i_j(\lambda r^{'}) Y_j^k(\theta^{'}, \phi^{'}) \tag{17}$$

where $(\rho^{'}, \alpha^{'}, \beta^{'})$ are the spherical coordinates of the vector $x - x_0$.

Definition 2.7. We denote by T_{LL}, the diagonal operator maping the harmonic expansion L_n^m to the shift harmonic expansion W_n^m.

Theorem 2.8. (Operator T_{LP}) Suppose that N strengths $(q_i)_{i\in[|1,N|]}$ are located at points $x_{i\in[|1,N|]}$ with spherical

coordinates $(\rho_i,\alpha_i,\beta_i)_{i\in[|1,N|]}$, respectively. Suppose further that the points $x_{i\in[|1,N|]}$ are located outside the sphere D of radius a centered at the origin. Then, for any point $x=(r,\theta,\phi)\in D$, the potential $\Phi(x)$ generated by the strengths $(q_i)_{i\in[|1,N|]}$ is equal to:

$$\Phi(x)=\sum_{j=0}^{p}\sum_{k=-j}^{j}L_j^k i_j(\lambda r)Y_j^k(\theta,\phi)$$

where

$$L_n^m=8\lambda\sum_{i=1}^{N}q_i k_n(\lambda\rho_i)Y_n^{-m}(\alpha_i,\beta_i)\;\forall(n,m)\in\mathbb{N}\times\mathbb{Z}\text{ avec }0\leq|\,m\,|\leq n. \tag{18}$$

2.1 The rotation based operators

In this section, we apply the rotation representation to factorize the operators T_{MM} and T_{LL}. For more details, we refer the reader to [6,42,43,44].

Theorem 2.9. We Consider the multipole expansion M_n^m, centered at $x_0=(\rho,\alpha,\beta)$ given by the theorem (2), we rotate the coordinate system so that the z-axis is aligned with the spherical angle β, we denote this operator $\mathscr{R}_z(\beta)$. Then we rotate the coordinate system so that the y-axis is aligned with the spherical angle α, we denote this operator $\mathscr{R}_z(\alpha)$, then there exist coefficients $\mathscr{R}(n,m,m',\alpha,\beta)$ such that:

$$\Phi(x)=\sum_{n=0}^{\infty}\sum_{m'=-n}^{n}\widetilde{M}_n^{m'}k_n(\lambda r')Y_n^m(\theta",\phi") \tag{19}$$

where $(r',\theta",\phi")$ are the new coordinates of x and

$$\widetilde{M}_n^{m'}=\sum_{m=-n}^{n}\mathscr{R}(n,m,m',\alpha,\beta)M_n^m. \tag{20}$$

Theorem 2.10. Consider the multipole expansion M_n^m, centered at $x_0=(\rho,\alpha,\beta)$ given by the theorem (2.1) which lies along the z-axis at a distance ρ from the origin. We obtain the new coefficients given by (2)

$$M_n^m=\sum_{n'=m}^{\infty}C_m^{n,n'}M_{n'}^m \tag{21}$$

where

$$C_m^{n,n'}=\sum_{k=m}^{min(n,n')}(\frac{1}{2})^k(-1)^{n'+k}(2n'+1)\frac{(n'-m)!(n+m)!(2k)!(\lambda\rho_z)^{-k}i_{n'+n+k}(\lambda\rho_z)}{(k+m)!(k-m)!(n'-k)!(n-k)!k!}. \tag{22}$$

Definition 2.11. We denote by T_{MM}^z, the diagonal operator maping the multipole expansion $M_{n'}^m$ to the shift multipole expansion M_n^m.

Theorem 2.12. Consider the multipole expansion L_n^m, centered at $x_0=(\rho,\alpha,\beta)$ given by the theorem (2.6) which lies

along the z-axis at a distance ρ from the origin. We obtain the new coefficients given by

$$L_n^m = \sum_{n'=m}^{\infty} C_m^{n,n'} L_{n'}^m \tag{23}$$

where

$$C_m^{n,n'} = \sum_{k=m}^{min(n,n')} (\frac{1}{2})^k (2n'+1) \frac{(n'-m)!(n+m)!(2k)!(\lambda\rho_z)^{-k} i_{n'+n+k}(\lambda\rho_z)}{(k+m)!(k-m)!(n'-k)!(n-k)!k!}. \tag{24}$$

Definition 2.13. We denote by T_{MM}^z, the diagonal operator maping the local expansion $L_{n'}^m$ to the shift multipole expansion L_n^m.

Formally, the scheme we have outlined corresponds to the factorizations the operators T_{MM} and T_{LL} with respect rotation by:

$$T_{MM} = \mathscr{R}_z(-\beta) \circ \mathscr{R}_y(-\alpha) \circ T_{MM}^z(\rho) \circ \mathscr{R}_y(\alpha) \circ \mathscr{R}_z(\beta) \tag{25}$$

and

$$T_{LL} = \mathscr{R}_z(-\beta) \circ \mathscr{R}_y(-\alpha) \circ T_{LL}^z(\rho) \circ \mathscr{R}_y(\alpha) \circ \mathscr{R}_z(\beta) \tag{26}$$

where (ρ, α, β) is the desired shifting direction.

2.2 Exponential expansions

The new generation of FMMs is based on introducing an additional approximation tool: exponential expansions let $Q = (x,y,z)$ and $P = (x_0,y_0,z_0)$ with $z > z_0$ and $r = \| Q - P \|$, then we have[45]):

$$k_0(\lambda r) = \frac{\pi}{2}\frac{e^{-\lambda r}}{\lambda r} = \frac{1}{4\lambda}\int_0^{\infty} e^{-(u+\lambda)(z-z_0)} \int_0^{2\pi} e^{i\sqrt{u^2+2u\lambda}((x-x_0)cos(\alpha)+(y-y_0)sin(\alpha))} d\alpha du \tag{27}$$

using quadrature formula in order to approximate this integral. For the outer u integral, we use the nodes and weights and for the inner α integral, we use the trapezoidal rule.

Lemma 2.14. let $Q = (x,y,z)$ and $P = (x_0,y_0,z_0)$ with $z > z_0$ and $r = \| Q - P \|$, Then,for any desired precision ε,we can write

$$\lambda \mid k_0(\lambda r) - \sum_{k=1}^{s(\varepsilon)} \frac{w_k}{M_k} \sum_{j=1}^{M_k} e^{-(u_k+\lambda)(z-z_0)} . e^{i\sqrt{u_k^2+2u_k\lambda}[(x-x_0).\cos(\alpha_{j,k})+(y-y_0).\sin(\alpha_{j,k})]} \mid < \varepsilon \tag{28}$$

with the flowing condition

$$1 \leq z - z_0 \leq 4 \text{ et } 0 \leq \sqrt{(x-x_0)^2+(y-y_0)^2} \leq 4\sqrt{2}. \tag{29}$$

where $\{w_k, k \in [|1 s(\varepsilon)|]\}$ are the weights, $\{u_k, k \in [|1, s(\varepsilon)|]\}$ are the nodes and the $s(\varepsilon)$ all depend on ε we use here quadrature formula given in [43](for further discussion and suggested methods of the degree approximation of signals in L_p-spaces [46,47] and in another side [50,51]) we describe in the tabular (1) some precision of $s(\varepsilon)$ and also for the corresponding total number of exponential $S_{exp} = \sum_{k=1}^{s(\varepsilon)} M_k$.
The following result provides an expansion of the form (28).

Corollary 2.15. Suppose that N charges $(q_i)_{i\in[|1,N|]}$ are located at points $X_{i\in[|1,N|]}$ with cartesian coordinates

	Précision(ε)	$s(\varepsilon)$	S_{exp}	p
$iprec = 0$	$1,6 \times 10^{-3}$	8	52	10
$iprec = 1$	$1,3 \times 10^{-6}$	17	258	19
$iprec = 2$	$1,1 \times 10^{-9}$	26	670	29

Table 1: *$s(\varepsilon)$ et S_{exp}, ainsi que du p correspondant, pour les trois precisions disponibles. Chaque precision est identifiee par une valeur de la variable iprec*

$(x_i, y_i, z_i)_{i\in[|1,N|]}$, respectively. Suppose further that the points $x_{i\in[|1,N|]}$ are located inside the cube C with unit volume centered at the origin. Then, for any point $X = (x, y, z) \in \mathbb{R}^3$,satisfies the conditions (29). The potential $\Phi(X)$ generated by the charges $(q_i)_{i\in[|1,N|]}$ and let Ψ_ε be defined by the formula:

$$\Psi_\varepsilon(X) \simeq \sum_{k=1}^{s(\varepsilon)} \sum_{j=1}^{M_k} \mathrm{W}(k, j) e^{-(u_k+\lambda)z} . e^{i\sqrt{u_k^2+2u_k\lambda}.(x\cos(\alpha_{j,k})+y\sin(\alpha_{j,k}))} \tag{30}$$

where $\mathrm{W}(k, j)$ are given by

$$\mathrm{W}(k, j) = \frac{w_k}{M_k} \sum_{l=1}^{N} q_l . e^{(u_k+\lambda)(z_l-z_0)} . e^{-i\sqrt{u_k^2+2u_k\lambda}.((x_l-x_0)\cos(\alpha_{j,k})+(y_l-y_0)\sin(\alpha_{j,k}))} \tag{31}$$

for all $k \in [|1, s(\varepsilon)|]$, $j \in [|1, M_k|]$ we difine $A = \sum_{l=1}^{N} |q_l|$. Then we have the folwing inequality:

$$|\Phi(X) - \lambda\Psi_\varepsilon(X)| < A_\varepsilon \tag{32}$$

In the FMM, two boxes are adjacent if they are at the same level of the hierarchy and have a boundary point. The *interaction list* of a box is defined to be the list of boxes on the same level of the hierarchy which are well separated from it but whose, parents are adjacent to its parent. For each box C in the interaction list of a box B, the FMM applies a far-field-to-local translation operator to convert the far-field expansion on B into a local expansion on C. To use plane wave representation for those translations, the *interaction list* subdivided into six lists, associated with the six coordinate directions $(+z, -z, +y, -y, +x, -x)$.

1. *Downlist*: boxes separated by at least one box in the -z-direction
2. *Uplist*: boxes separated by at least one box in the +z-direction.
3. *Northlist*: boxes separated by at least one box in the +y-direction, and are not contained in the *Uplist* or *Downlist*.
4. *Southlist*: boxes separated by at least one box in the -y-direction, and are not contained in the *Uplist* or *Downlist*.
5. *Eastlist*: boxes separated by at least one box in the +x-direction, and are not contained in the *Uplist*, *Downlist*, *Northlist* or *Southlist*.
6. *Westlist* : boxes separated by at least one box in the in the *Uplist*, *Downlist*, *Northlist* or *Southlist*.

Remark 2.16. It is easy to chek for two boxes, B, C, that:

$$\begin{aligned} c \in Uplist(B) &\Leftrightarrow B \in Downlist(C) \\ c \in Northlist(B) &\Leftrightarrow B \in Southlist(C) \\ c \in Eastlist(B) &\Leftrightarrow B \in Westlist(C) \end{aligned} \tag{33}$$

and if we choose two boxes B and C, if $C \in Uplist(B)$, then for any point $X_0 = (x_0, y_0, z_0) \in B$ and $X = (x, y, z) \in C$ we have

$$1 \le z - z_0 \le 4 \ \text{ et } 0 \le \sqrt{(x-x_0)^2 + (y-y_0)^2} \le 4\sqrt{2}. \tag{34}$$

3 Conversion between exponential and partial-wave expansions

Expansions of the form (30) will be referred to as exponential expansions. Their main utility is that translation takes a particularly simple form.

Theorem 3.1. Suppose that a box B of volume d^3 centered at the origin and a box B. Suppose that $B \in Downlist(C)$. and M_n^m ($\forall (n,m) \in \mathbb{N} \times \mathbb{Z}$ avec $0 \leq \mid m \mid \leq n$) be the multipole expansion B, see the theorem (2)). for any point $X \in C$

$$\Phi(X) \simeq \lambda \sum_{k=1}^{s(\varepsilon)} \sum_{j=1}^{M_k} \mathrm{W}(k,j) e^{-(u_k+\lambda)(\frac{z}{d})} . e^{i\sqrt{u_k^2+2u_k\lambda}.((\frac{x}{d})\cos(\alpha_{j,k})+(\frac{y}{d})\sin(\alpha_{j,k}))} \tag{35}$$

where (x,y,z) are the Cartesian coordinates of X and $\mathrm{W}(k,j)$ for all $k \in [|1, s(\varepsilon)|]$, $j \in [|1, M_k|]$ is given by :

$$\mathrm{W}(k,j) = \frac{\pi w_k}{2d\lambda M_k} \sum_{m=-p}^{p} i^{|m|} . e^{im\alpha_{j,k}} \sum_{n=|m|}^{p} M_n^m \sqrt{\frac{2n+1}{4\pi}} \sqrt{\frac{(n-|m|)!}{(n+|m|)!}} P_n^{|m|}(\frac{\lambda+u_k}{\lambda}) \tag{36}$$

Definition 3.2. We denote by C_{MX} the linear operator maping the coefficients in harmonic expansion M_n^m to the coefficient in the exponential expansion $\mathrm{W}(k,j)$.

Theorem 3.3. We view the formula (30) as an expansion centered at the origin for $X = (x,y,z)$. Then for any $X_0 = (x_0, y_0, z_0) \in \mathbb{R}^3$ we have

$$\Phi(X) \simeq \sum_{k=1}^{s(\varepsilon)} \sum_{j=1}^{M_k} \mathrm{V}(k,j) . e^{-(u_k+\lambda)(z-z_0)} . e^{i\sqrt{u_k^2+2u_k\lambda}.((x-x_0)\cos(\alpha_{j,k})+(y-y_0)\sin(\alpha_{j,k}))} \tag{37}$$

where

$$\mathrm{V}(k,j) = \mathrm{W}(k,j) . e^{-(u_k+\lambda)z_0} . e^{i\sqrt{(u_k^2+2u_k\lambda)}x_0\cos(\alpha_{j,k})+y_0\sin(\alpha_{j,k}))} \tag{38}$$

for $k \in [|1, s(\varepsilon)|]$ and $j \in [|1, M_k|]$.

Definition 3.4. we denote by $D_{\widetilde{bc}}$ the diagonal operator maping the exponential expansion $\mathrm{W}(k,j)$ to the shift exponential expansion $\mathrm{V}(k,j)$.

Theorem 3.5. Suppose that N charge of strengths $(q_i)_{i\in[|1,N|]}$, located at points $x_{i\in[|1,N|]}$ are inside box B of volume d^3 centered at the origin. Then for any point $X = (x,y,z) \in Uplist(B)$, the potential $\Phi(X)$ satisfies the inequality

$$\Phi(X) \simeq \lambda \sum_{k=1}^{s(\varepsilon)} \sum_{j=1}^{M_k} \mathrm{W}(k,j) e^{-(u_k+\lambda)(\frac{z}{d})} . e^{i\sqrt{u_k^2+2u_k\lambda}.((\frac{x}{d})\cos(\alpha_{j,k})+(\frac{y}{d})\sin(\alpha_{j,k}))} \tag{39}$$

Then there exists an integer p such that

$$\Phi(X) \simeq \sum_{n=0}^{p} \sum_{m=-n}^{n} L_n^m i_n(r) Y_n^m(\theta,\phi) \tag{40}$$

where (r,θ,ϕ) are the spherical coordinates of X and we have

$$L_n^m = (-1)^n i^{|m|}\sqrt{4\pi}\sqrt{2n+1}\sqrt{\frac{(n-|m|)!}{(n+|m|)!}}\sum_{k=1}^{s(\varepsilon)} P_n^{|m|}(\frac{u_k+\lambda}{\lambda})\sum_{j=1}^{M_k} \mathrm{W}(k,j).e^{im\alpha_{j,k}} \tag{41}$$

for $n \in [|0,p|]$ and $j \in [|-n,n|]$.

Definition 3.6. We denote by C_{XL} the linear operator maping the coefficients in an exponential expansion $\mathrm{V}(k,j)$ to the coefficient in the harmonic expansion L_n^m.

Remark 3.7. Suppose that B and C be two boxes, if $C \in Uplist(B)$. Then the translation operator T_{ML} given in the theorem (2.4) which converts a multipole expansion centered in B to a local expansion centered in C can be write as

$$T_{ML} = C_{XL} \circ D_{\widetilde{bc}} \circ C_{LX}. \tag{42}$$

Remark 3.8. The cost of single multipole-to-local translation using the factorisation of (42) is

$$\mathscr{O}(2p^2 + 2p^2 s(\varepsilon) + 2pS_{exp}) = \mathscr{O}(2p^2 + 4p^3) = \mathscr{O}(p^3)$$

since $s(\varepsilon) \approx p$ and $S_{exp} \approx p^2$. In the FMM, a large number of multipôle-to-local translation is of $\mathscr{O}(p^3)$ or $\mathscr{O}(p^4)$ but in the new FMM, a large number of multipôle-to-local of exponential translation, costs $\mathscr{O}(p^2)$(FIG.1.)

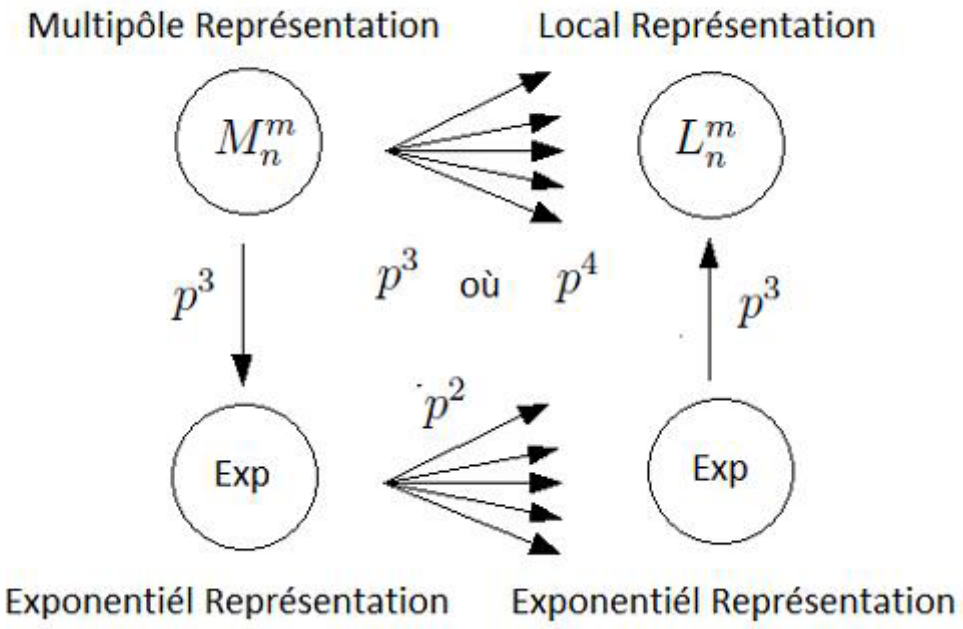

Fig. 1: In the FMM, using the operator T_{ML}, costing $\mathscr{O}(p^3)$ or $\mathscr{O}(p^4)$ but in the new FMM using $\mathscr{D}_{\widetilde{bc}}$, costing $\mathscr{O}(p^2)$

.

The decomposition (42) of the operator T_{ML} is valid only when box $C \in Uplist(B)$. This corresponds to the factorization for all other case:
if $c \in Downlist(b)$

$$T_{ML}^{Down} = \mathscr{R}_y(-\pi)C_{XL}D_{\widetilde{bc}}C_{MX}\mathscr{R}_y(\pi) \tag{43}$$

if $c \in Eastlist(b)$

$$T_{ML}^{East} = \mathscr{R}_y(-\pi/2)C_{XL}D_{\widetilde{bc}}C_{MX}\mathscr{R}_y(\pi/2) \tag{44}$$

if $c \in Westlist(b)$

$$T_{ML}^{West} = \mathscr{R}_y(\pi/2)C_{XL}D_{\widetilde{bc}}C_{MX}\mathscr{R}_y(-\pi/2) \tag{45}$$

if $c \in Northlist(b)$

$$T_{ML}^{North} = \mathscr{R}_y(-\pi/2)\mathscr{R}_z(-\pi/2)C_{XL}D_{\widetilde{bc}}C_{MX}\mathscr{R}_y(\pi/2)\mathscr{R}_z(\pi/2) \tag{46}$$

if $c \in Southlist(b)$

$$T_{ML}^{South} = \mathscr{R}_y(\pi/2)\mathscr{R}_z(-\pi/2)C_{XL}D_{\widetilde{bc}}C_{MX}\mathscr{R}_y(-\pi/2)\mathscr{R}_z(\pi/2) \tag{47}$$

where $\mathscr{R}_y$ and $\mathscr{R}_z$ the operators defined by the theorem (2.9)

Definition 3.9. We denote T_{ML}^{Up} the operator given by the theorem(3.3).
Then, for $Dir \in \{Up, Down, East, West, North, South\}$

$$T_{ML}^{Dir} = \mathscr{Q}^{Dir}D_{\widetilde{bc}}\mathscr{P}^{Dir} \tag{48}$$

and

$$\mathscr{Q}^{Up} = C_{XL}$$

$$\mathscr{P}^{Up} = C_{MX}$$

$$\mathscr{Q}^{Down} = \mathscr{R}_y(-\pi)C_{XL}$$

$$\mathscr{P}^{Down} = C_{MX}\mathscr{R}_y(\pi)$$

etc.

Now, we describe the algorithm of new FMM.

Comments

–N : The number of particles.
–s: The average number of particles per box.
–The number of boxes at the finest level is then 8^n.
–$H \approx \log_8(N)$: The number of rafinement levels .
–$\mathscr{M}_{l,i}$: The multipole expansion for box i at level l.
–$\mathscr{L}_{l,i}$: The locale expansion for box i at level l.
–p : The order of the multipole expansion.

–W_i : The "outgoing" exponential expansion for the box i.
–V_i : The "incoming" exponential expansion for the box i
–$p(i)$: The parent of the box i.
–$F(i)$: The children of the box i.
–$V(i)$: The neighbor boxes of the box i.

Algorithm

Upward Pass:

step 1

Do for $i = 1$ to 8^H
In applying T_{PM} by using Theorem (2.1)to calcul $\mathscr{M}_{H,i}$.
End do

step 2

Do for $l = H-1$ to 0
Do for $i = 1$ to 8^l
$\mathscr{M}_{l,i} = \sum_{k\in F(i)} T_{MM}(\mathscr{M}_{l+1,k})$ In applying T_{MM}, use the factorisation (25)).
End do
End do

Downward Pass:

Initialization

$$(\mathscr{L}_{1,1},\mathscr{L}_{1,2},\mathscr{L}_{1,3},\mathscr{L}_{1,4},\mathscr{L}_{1,5},\mathscr{L}_{1,6},\mathscr{L}_{1,7},\mathscr{L}_{1,8}) = (0,0,0,0,0,0,0,0)$$

step 3*A*

Do for $l = 2$ to 8^H
Do for $i = 1$ to 8^l
In applying T_{LL}
use the factorisation (26).
$\mathscr{L}_{l,i} = T_{LL}(\mathscr{L}_{l-1,p(i)})$
End do

step 3*B*

Do for $Dir = Up, Down, East, West, North, South$
Do for $i = 1$ à 8^l
$W_i = \mathscr{P}^{Dir}\mathscr{M}_{l,i}$
End do
Do for $i = 1$ à 8^l
$V_i = \sum_{k\in -Dirlist(i)} D_{\widetilde{ki}} W_k$
$\mathscr{L}_{l,i} = \mathscr{L}_{l,i} + \mathscr{Q}^{Dir} V_i$
End do
End do
End do

Direct calculation:

Do for $i = 1$ à 8^H
for each particle x_j in each box i at the finest level n.

$\mathscr{V}_i(x) = \sum_{j\in V(i)} \sum_{k/x_k\in j} q_k \frac{e^{-\lambda\|x-x_k\|}}{\|x-x_k\|}$

End do

End do

Evaluation:

Do for $i = 1$ to 8^H

for each particle x_j in each box i at the finest level n.

$\Phi(x_j) = \mathscr{V}_i(x_j) + T_{LP}(\mathscr{L}_{l,i})$ In applying T_{LP} via the theorem (2)

End do

End do

Complexity

Upward Pass: Step1 require Np^2 work, Step2 require p^3N/s.
Then the total operation count is $Np^2 + p^3N/s$.

Downward Pass: In the step3B, the operator $\mathscr{P}^{Dir}$ and $\mathscr{Q}^{Dir}$ require a total $20p^3N/s$ work, in addition $D_{\tilde{ki}}$ require $40p^2N/s$ work, while the step3A require approximately $2p^3N/s$. Then this phase require a total approximately

$$22p^3N/s + 40p^2N/s$$

Direct Calculation: Require $27Ns$ work

Evaluation : Require Np^2 work

The total operation count of this algorithm is

$$2Np^2 + 27Ns + 23p^3N/s + 40p^2N/s$$

with $s = p$ we have.

$$25Np + 67Np^2$$

4 Numerical results

The algorithm described above has been implemented using Fortran. We assume that the molecules are distributed randomly but uniformly in the cylinder of radius 0.5 and height 1 centered at the origin and assign random charges(Tab.2). In the (Tab.3) the 10 first charges(points) and their corresponding potential $\Phi_{FMM}(x)$(Results for the FMM) values are presented (where we set the parameters $p = 9$, $s = 9$, $\lambda = 0.1$ and $N = 1000$).

From the graph (Fig.2), we can see that our methods is faster than the direct method. We show on the figure (Fig.3) the results for the times obtained with different level , which were a perfectly decreasing function versus the levels. We plot the max value of error between the FMM and the direct method in the (Fig.4). We have demonstrated from the graph (Fig.5) that in the algorithm of the FMM we used to much more the far-interaction than the near-interaction when the level is increasing.

charges	x	y	z	strengths
x_1	-4.865305×10^{-2}	-0.116861	-8.534741×10^{-2}	-0.432231
x_2	4.931268×10^{-2}	-1.569199×10^{-2}	0.265337	-0.468166
x_3	-4.690647×10^{-2}	0.432640	0.387879	9.132957×10^{-2}
x_4	-2.122139×10^{-3}	0.333354	-0.313664	0.235652
x_5	-3.849470×10^{-2}	0.198658	-0.144396	0.138299
x_6	4.082102×10^{-2}	-0.205999	-0.235028	-0.122506
x_7	4.162001×10^{-3}	-0.490718	0.499465	-0.487098
x_8	3.424971×10^{-2}	0.352470	-3.298902×10^{-2}	-0.446392
x_9	4.767475×10^{-2}	-0.303245	0.356972	-0.355786
x_{10}	3.006620×10^{-2}	0.229397	0.485790	-0.316594

Table 2: *The first* 10 *charges with Cartesian coordinates* (x,y,z) *and the corresponding strengths.*

	Φ_{Direct}	Φ_{FMM}
x_1	-501.21302400160931	-501.19261117960400
x_2	-512.57062662156181	-512.71830777778700
x_3	-358.64606129257987	-358.66337264124934
x_4	-75.771611680888114	-75.846862742769758
x_5	-316.55716166806576	-316.55240570929720
x_6	-385.06053121793047	-385.05057788179772
x_7	90.132160675063830	90.130162454275805
x_8	-468.81730704742853	-468.84596793501078
x_9	-20.470850268893468	-20.533753063751568
x_{10}	-668.42206457284703	-668.45932308693079

Table 3: *The* 10 *first charges(points) and their corresponding potential* $\Phi_{FMM}(x)$.

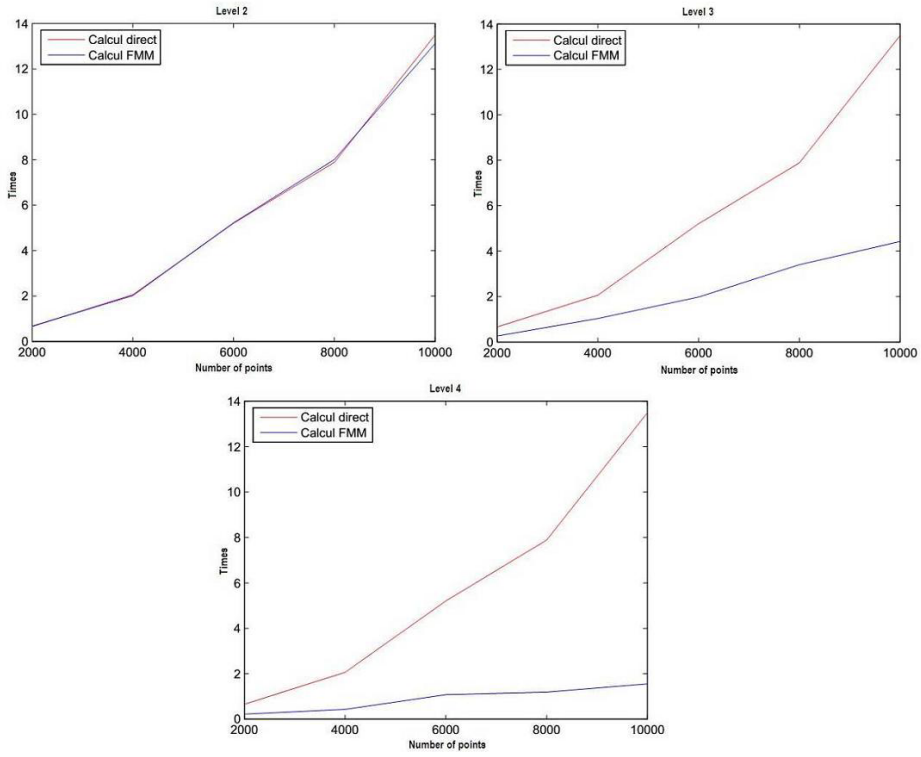

Fig. 2: Graph of times versus number of points.

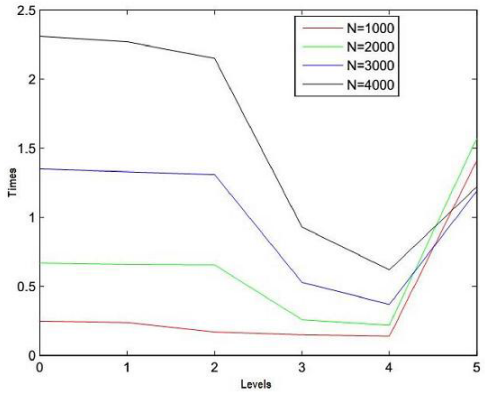

Fig. 3: Graph of times versus the levels of Octree.

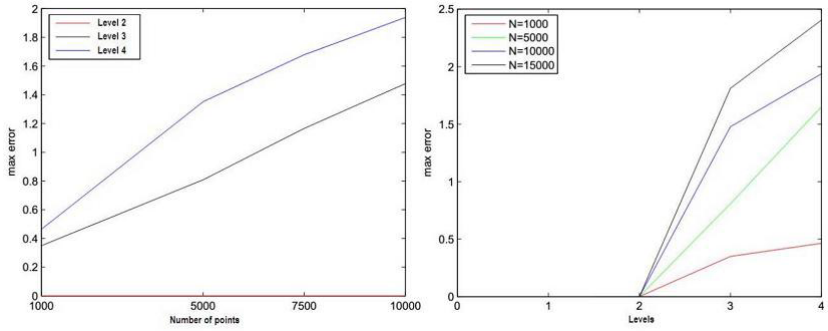

Fig. 4: Graph of max values of error versus the number of points and the levels of Octree.

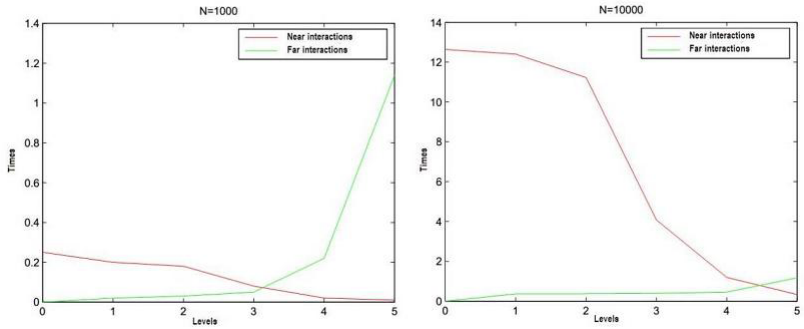

Fig. 5: Graph of the times of calcul of the far-interractions and near-interactions versus the levels of Octree.

5 Conclusions

We have presented an investigation on coupling available algorithms of the new fast multipole method for the linearized Poisson-Boltzmann equation for the purposes to accelerate the product matrix-vector in three dimensions. We applied the FMM to points on the surface of the cylinder of radius 0.5 and height 1 centered at the origin. With this approach we achieve fast convergence for our test cases. One important aim of this paper was to identify and elucidate the remaining issues that need to be solved in order to develop this approach into a fully general solver.

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