

Telescoping Fast Multipole Methods Using Chebyshev Economization

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Chebyshev polynomials of the first kind are applied to telescope both the far-field multipole expansions and the near-field Taylor series expansions used in solving large N -body problems via fast multipole methods. The technique is demonstrated for pairwise-additive, $1/r$ interparticle potentials in Cartesian coordinates, and a general *Mathematica*® package is provided to derive the modified expansion coefficients symbolically. Accelerated convergence and more uniform error can be achieved without additional computations during runtime. Hence the telescoped series require fewer expansion terms for a given accuracy requirement, saving considerable computational expense over conventional fast multipole implementations. © 1995 Academic Press, Inc.

1. INTRODUCTION

Over the last decade considerable effort and progress have been made towards efficiently implementing large N -body computer simulations. The more recent approaches replace groups of distant particles by moments of charge (or mass) and compute the interactions between groups using this approximation. Appel [1] and Barnes and Hut [2] introduced $O(N \log N)$ algorithms using hierarchical tree structures to classify particle interactions and low-order multipole expansions to compute far-field interactions. Greengard and Rokhlin [3–7] and Zhao [8] implemented both far-field and local expansions resulting in $O(N)$ fast multipole methods (FMM) for Coulombic and gravitational potentials, respectively. These multipole methods considerably improve computational efficiency and accuracy. Subsequently, numerous investigators have reported efficient implementations in a variety of particle simulations; however, few have actually extended the fast multipole method itself.

Lustig *et al.* [9] implemented the FMM in molecular dynamics for complex particle interactions such as: soft-sphere, Lennard–Jones, Morse and Yukawa potentials. Ding *et al.* [10] combined Coulomb and London interactions, but achieved only limited accuracy. More recently Shimada *et al.* [11, 12] developed a combined particle–particle and particle–mesh/multipole expansion technique. In all the aforementioned methods, increased accuracy can be achieved by increasing the number of expansion terms retained in the multipole or local series, but always at a significant increase in computational expense.

There is considerable motivation to improve the convergence of FMM expansions. Low-order expansions, such as those truncating at the quadrupolar terms, often provide error levels in potential gradients that are unacceptable for stable, long-time simulations. Unfortunately, the computational expense of the FMM increases with the number of expansion terms, p , scaling as $O(p^4)$ in spherical coordinates and $O(p^6)$ in Cartesian coordinates. In addition, most computational shortcuts such as “supernodes” [8], or parental conversion in interactive lists, seem only to degrade FMM accuracy. Furthermore, multipole and Taylor series approximations generally exhibit the same, uneven error distribution that can also result in cumulative, systematic artifacts in long-time dynamical simulations.

In this work we apply Chebyshev economization to both far-field multipole expansions and near-field Taylor series expansions used in solving large N -body problems involving pairwise-additive, interparticle potentials. Chebyshev economization is a standard technique to approximate efficiently polynomial representations and can be found in numerical analysis texts, e.g., [13–14]. Briefly, when polynomial series are expressed using Chebyshev polynomials, some of the high-order Chebyshev polynomials can be dropped with the assurance that the error involved is less than a prescribed tolerance. The truncated series can then be retransformed to a polynomial

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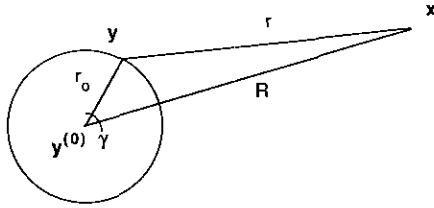


FIG. 1. Geometry of far-field.

with fewer terms than the original, but with modified coefficients. The resulting approximation tends to yield the smallest number of terms that will supply an accuracy within the prescribed tolerance. Furthermore, the maximum error from the untruncated series is minimized over the entire domain of application, providing more uniform error. The technique is applicable to expansions in any coordinate system. We do not repeat a description of the FMM since details are available from original [3–8] and secondary [10, 15, 16] literature. In the following we demonstrate the economization technique for simple $1/r$ potentials for Zhao's FMM framework [8] in three-dimensional, Cartesian coordinates.

2. TELESCOPING THE FAR-FIELD MULTIPOLE EXPANSION

One of the initial steps in the FMM is to compute the multipole moments of mass (or charge) at a point $\mathbf{y}^{(0)}$ due to particles inside a region bounded by a sphere centered at $\mathbf{y}^{(0)}$ of radius r_0 . For the purpose of illustration, we need to consider only one particle at position, \mathbf{y} , on the sphere; see Fig. 1. The distances r and R are from the position \mathbf{x} to the particle and sphere center, respectively. The potential, $\Phi = 1/r$, at a point, \mathbf{x} , well-separated from $\mathbf{y}^{(0)}$ due to the particle is given by the following multiple expansion (1):

$$\frac{1}{r} = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \sum_{k=0}^{\infty} a_{ijk} \frac{\partial^{i+j+k}}{\partial x_1^i \partial x_2^j \partial x_3^k} \left(\frac{1}{R} \right). \quad (1)$$

In the above x_i ($i = 1, 2, 3$) indicate the Cartesian components of \mathbf{x} and the coefficients are given by

$$a_{ijk} = (-1)^{i+j+k} \frac{r_0^{i+j+k}}{i! j! k!} v_1^i v_2^j v_3^k, \quad (2)$$

where v_i ($i = 1, 2, 3$) denote the direction cosines between $\overline{\mathbf{y}^{(0)}\mathbf{y}}$ and the coordinate axes. In the FMM we truncate the far-field expansion (1) to a tetrahedral summation

$$\Phi(\mathbf{x}) = \sum_{n=0}^p \sum_{\substack{i,j,k=0 \\ i+j+k=n}} a_{ijk} \frac{\partial^{i+j+k}}{\partial x_1^i \partial x_2^j \partial x_3^k} \left(\frac{1}{R} \right) + \varepsilon \quad (3)$$

and compute the coefficients a_{ijk} up to order p . The truncation error, ε , is small for $r_0/R \ll 1$ and is bounded by

$$|\varepsilon| \leq \left(\frac{r_0}{R} \right)^{p+1}, \quad (4)$$

as proven earlier [8].

It is most common in FMM implementations to define the minimum distance of the far-field using $r_0/R \leq \frac{1}{2}$. FMM-savvy readers recognize this definition (i) expresses the choice of defining a node's far-field as those nodes which are not included in the 26 immediately neighboring nodes and (ii) involves a compromise between FMM accuracy for a given value of p and computational effort spent computing near-field interactions directly. In fact, the far-field can be defined by $r_0/R \leq 1/(n+1)$, $n = 1, 2, 3, \dots$. To illustrate our method for improving the convergence of (3) over the chosen range, we use the far-field criterion $r_0/R \leq \frac{1}{2}$.

The series in Eq. (1) can also be represented using Legendre polynomials, P_n , e.g., see [17], as

$$\frac{1}{(r/R)} = \sum_{n=0}^{\infty} P_n(\cos \gamma) \left(\frac{r_0}{R} \right)^n. \quad (5)$$

Since in practice we use only $r_0/R \leq \frac{1}{2}$, we define an expanded coordinate scale, ρ ,

$$\rho \equiv 2 \frac{r_0}{R}. \quad (6)$$

Notice that $|\rho| \leq 1$, which sets the appropriate interval for telescoping the series using Chebyshev polynomials. Introducing (6) into (5), we can always find a set of coefficients, \overline{C}_n , and a truncation order, p , for any desired, prescribed truncation error, ε , satisfying

$$\frac{1}{(r/R)} = \sum_{n=0}^{\infty} P_n(\cos \gamma) \left(\frac{\rho}{2} \right)^n = \sum_{n=0}^p \frac{\overline{C}_n}{2^n} T_n[P_n(\cos \gamma) \rho^n] + \varepsilon. \quad (7)$$

Here $T_n[x]$ is the n th-order Chebyshev polynomial of the first kind. Although tedious, rewriting a polynomial expansion into an equivalent Chebyshev polynomial expansion is straightforward and is computed symbolically [18] by the subroutine ChebyshevSeries in the Appendix. Since the maximum magnitude of any Chebyshev polynomial in $[-1, 1]$ is unity, the appropriate truncation can be predicted for the prescribed error from

$$\varepsilon \leq \sum_{n=p+1}^{\infty} \frac{\overline{C}_n}{2^n}. \quad (8)$$

As it is not practical to carry the error calculation in (8) to an

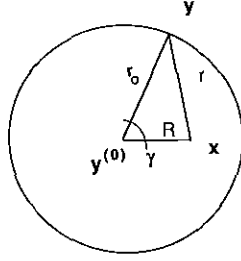


FIG. 2. Geometry of near-field.

infinite number of terms, the summation is continued until the highest order term is a sufficiently small contribution to the sum. Once the appropriate truncation order is established, the series can be recast as a series in Legendre polynomials with modified coefficients, C_n ,

$$\frac{1}{(r/R)} = \sum_{n=0}^p C_n P_n(\cos \gamma) \left(\frac{r_0}{R}\right)^n + \varepsilon. \quad (9)$$

The aforementioned steps are performed by the operator `TelescopeSeries[]` in the Appendix. The desired power series coefficients C_n are printed as the results.

Finally, we must recover the modified far-field coefficients to compute. The Legendre polynomials in (9) are replaced using the identity [17]

$$P_n(\cos \gamma) = (-1)^n \frac{R^{n+1}}{n!} \frac{\partial^n}{\partial r_0^n} \left(\frac{1}{R}\right) \quad (10)$$

and after using (6) we obtain

$$a_{ijk} = (-2)^{i+j+k} \frac{C_{(i+j+k)} r_0^{i+j+k}}{i! j! k!} v_1^i v_2^j v_3^k \quad (11)$$

which is the desired result for the FMM implementation.

3. TELESCOPING THE NEAR-FIELD TAYLOR EXPANSION

An $O(N)$ FMM [3–8] also makes use of a near-field Taylor expansion of the interparticle potential to convert the above far-field multipole coefficients, a_{ijk} , into near-field coefficients, b_{ijk} , at each hierarchical level. Figure 2 illustrates the situation in which the potential field $\Phi(\mathbf{x})$ is to be computed near the center of a sphere located at $\mathbf{y}^{(o)}$ due to a mass (or charge) distribution at point \mathbf{y} . Equation (12) follows directly from the Law of Cosines:

$$\frac{1}{r} = 1 / r_0 \sqrt{1 + \left[\left(\frac{R}{r_0}\right)^2 - 2 \left(\frac{R}{r_0}\right) \cos \gamma \right]}. \quad (12)$$

The quantity in the brackets is small in the near-field and is replaced by the variable ξ , $|\xi| < 1$:

$$\frac{1}{(r/r_0)} = \frac{1}{\sqrt{1 + \xi}}. \quad (13)$$

The original Cartesian FMM implementation [8] expands (13) directly in terms of ξ , resulting in

$$\frac{1}{(r/r_0)} = \sum_{n=0}^{\infty} \binom{-\frac{1}{2}}{n} \xi^n. \quad (14)$$

As described in the previous section, it is common practice in FMM implementation to define the minimum distance of the far-field using $r_0/R \leq \frac{1}{2}$, so the near-field is defined using $\xi \leq \frac{1}{2}$. Since in practice we will only use the range $|\xi| \leq \frac{1}{2}$, we define expanded coordinate $\rho \equiv 2\xi$, $|\rho| \leq 1$, such that

$$\frac{1}{(r/r_0)} = \sum_{n=0}^{\infty} \binom{-\frac{1}{2}}{n} \left(\frac{\rho}{2}\right)^n. \quad (16)$$

This power series can be telescoped by Chebyshev economization using steps similar to those described in the previous section. First, the Taylor series expansion is created, in this case using the *Mathematica*[®] operators `Normal[Series[]]`. Second, the operator `ChebyshevSeries[]` creates an equivalent expansion in terms of Chebyshev polynomials with coefficients, \bar{C}_n . Third, the operator `TelescopeSeries[]` determines the minimum truncation order, p , for a prescribed error, ε , over $|\rho| \leq 1$:

$$\frac{1}{(r/r_0)} = \sum_{n=0}^{\infty} \binom{-\frac{1}{2}}{n} \left(\frac{\rho}{2}\right)^n = \sum_{n=0}^p \bar{C}_n T_n[\rho] + \varepsilon. \quad (17)$$

Next, the truncated Chebyshev series is recast in terms of the equivalent power series with coefficients, C_n :

$$\frac{1}{(r/r_0)} = \sum_{n=0}^p C_n \xi^n + \varepsilon. \quad (18)$$

After application of some trigonometric identities as well as the multinomial and binomial theorems following [8], we obtain

$$\frac{1}{r} = \sum_{n=0}^p \sum_{\substack{i,j,k=0 \\ i+j+k=n}}^n b_{ijk} (x_1 - y_1^{(o)})^i (x_2 - y_2^{(o)})^j (x_3 - y_3^{(o)})^k + \varepsilon. \quad (19)$$

$$b_{ijk} = \frac{(-1)^{i+j+k}}{r_0^{1+i+j+k}} \sum_{\alpha=0}^{\lfloor i/2 \rfloor} \sum_{\beta=0}^{\lfloor j/2 \rfloor} \sum_{\gamma=0}^{\lfloor k/2 \rfloor} C_{(i-\alpha+j-\beta+k-\gamma)}$$

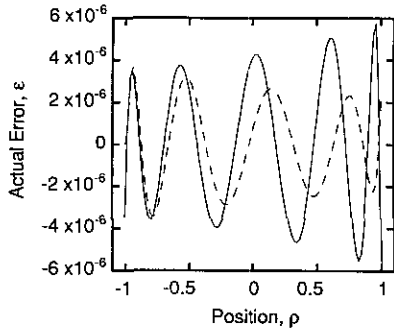


FIG. 3. Absolute error as a function of position for the telescoped far-field multipole expansion $p = 9$ (solid line) and telescoped near-field Taylor series expansion $p = 8$ (dashed line). The prescribed error tolerance is $\epsilon = 10^{-5}$ in both cases.

$$\begin{aligned} & \times \frac{(i - \alpha + j - \beta + k - \gamma)!}{(i - \alpha)!(j - \beta)!(k - \gamma)!} \\ & \times \binom{i - \alpha}{\alpha} \binom{j - \beta}{\beta} \binom{k - \gamma}{\gamma} \\ & \times (2v_1)^{i-2\alpha} (2v_2)^{j-2\beta} (2v_3)^{k-2\gamma}, \end{aligned} \quad (20)$$

which are the desired results for the FMM implementation.

4. RESULTS

Two example calculations are considered for a prescribed error tolerance of 10^{-5} using only adjacent neighbors to define the FMM near- and far-fields. The telescoped far-field multipole expansion requires a truncation order of $p = 9$, whereas the original expansion requires $p = 16$ to achieve the same error tolerance. The solid line in Fig. 3 illustrates the actual error, ϵ , as a function of position, ρ , using Eq. (17). Although the $p = 8$ truncation error exceeds 10^{-5} , the actual $p = 9$ truncation error remains less than 6×10^{-6} in absolute magnitude within $|\rho| \leq 1$. The telescoped near-field Taylor expansion requires a truncation order of $p = 8$ and the actual error as a function of position is illustrated by the dashed line in Fig. 3. The error remains less than 4×10^{-6} , indicating that the telescoped near-field Taylor expansion is slightly more efficient than the telescoped far-field multipole expansion. If we were to implement the telescoped FMM with $p = 9$ for both expansions, we would expect a $(16/9)^6$, or roughly 32-fold, reduction in execution time compared to the original FMM with the same 10^{-5} error tolerance. This advantage increases exponentially as the prescribed error tolerance is further decreased.

Telescoping the FMM far-field and near-field series provides a considerable convergence advantage. In this communication we define a FMM near-field using $R/r_o \leq \frac{1}{2}$, i.e., only

immediately adjacent neighbors. More rapid convergence would be obtained in both the original and telescoped FMM by extending the near-field boundary. Figure 4 illustrates the maximum absolute error in the near-field and far-field domains for the original and telescoped FMM. The near-field and far-field expansion errors are equivalent for various expansion orders in the original FMM [8], although the Chebyshev economization technique discussed here is slightly more efficient for the near-field expansion. As there is no error associated with the FMM translation operators [8], the entire FMM calculation accuracy would be limited by the telescoped far-field multipole expansion.

For completeness we provide some useful numerical values of economized coefficients in Tables I and II. Table I summarizes the C_n coefficients for equation (11) and maximum absolute errors for various truncations of the telescoped far-field multipole expansion. Table II summarizes the C_n coefficients for Eq. (20) and maximum absolute errors for various truncations of the telescoped near-field expansion. These coefficients were obtained by approximating the infinite sums in Eqs. (7) and (17) with 100-term expansions as input to the operator TelescopeSeries[].

5. CONCLUSION

These results suggest that Chebyshev economization can markedly improve the FMM. In practice the far-field and near-field expansion coefficients are precomputed and stored during the initialization section of a high-performance N -body code. Therefore, the substantially increased accuracy is obtained without increased run-time cost and requires only minor changes to an existing code. In forthcoming publications we shall investigate aspects of applying telescoped multipole methods, TMM, to physical problems.

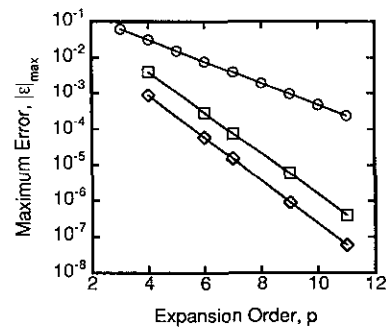


FIG. 4. Maximum error as a function of expansion order for the untelescoped FMM [8] (open circles), telescoped far-field multipole expansion (open squares), and telescoped near-field Taylor series expansion (open diamonds). In these cases the FMM near-field is defined using only immediately adjacent neighbors.

TABLE I
Far-Field Telescoped Coefficients, C_n , in Eq. (11) and Maximum Error for Truncation Order p

p= Error= n	4 4.0×10^{-3} C_n	6 3.0×10^{-4} C_n	7 7.5×10^{-5} C_n	9 6.0×10^{-6} C_n	11 4.0×10^{-7} C_n
0	+1.00079744664	+0.999942745907	+0.999942745907	+1.00000411066	+0.999999704868
1	+0.485518166354	+0.501467099244	+0.499863984637	+0.500011968359	+0.499998982550
2	+0.236379510021	+0.251764123298	+0.251764123298	+0.249800451233	+0.250020740781
3	+0.177711982884	+0.113916251322	+0.126741168178	+0.124768051887	+0.125027768076
4	+0.0952355645984	+0.0542099291921	+0.0542099291921	+0.064028289519	+0.0622659731303
5		+0.0510365852497	+0.0253867515388	+0.0324899701844	+0.0310355595247
6		+0.0273504236042	+0.0273504236042	+0.0116410470812	+0.0165755329694
7			+0.0146570478348	+0.00518608964067	+0.00851045686284
8				+0.00785468826151	+0.00221527581782
9				+0.00420931475294	+0.00088494753078
10					+0.00225576497748
11					+0.00120886080806

APPENDIX: Mathematica® PACKAGE

(*ChebyshevSeries returns a table of arithmetic coefficients, C_n , for the series of Chebyshev polynomials, $T_n(x)$, which is equivalent to the input polynomial, *polyinput*, in terms of the independent variable, x .)

```
ChebyshevSeries[polyinput_, x_] :=
Block[{n, Cn, CnTable, cnpoly, Pn,
polynomial},
polynomial = polyinput;
CnTable = Table[0, {i, 0,
Exponent[poly, x]}];
For[n = Exponent[poly, x], n > 0, n--,
cnpoly = ChebyshevT[n, x];
Cn = Coefficient[cnpoly, x, n];
Pn = Coefficient[polynomial, x, n];
polynomial = Apart[polynomial -
(Pn*cnpoly)/Cn];
CnTable[[n + 1]] = Pn/Cn;
Null];
```

```
CnTable[[1]] = polynomial;
Return[Simplify[CnTable]];
Null]
```

(* TelescopeSeries accepts a normal series, *seriesinput*, to telescope in terms of a single independent variable, x , with a user-requested maximum error, *error*, and returns a series telescoped over the range $|x| \leq 1$.)

```
TelescopeSeries[seriesinput_, x_, error_] :=
Block[{cumError = 0, degr, Ctable,
Stable, Ttable, n, poly},
poly = Collect[Expand[seriesinput], x];
degr = Exponent[poly, x];
Ctable = ChebyshevSeries[poly, x];
For[n = 0, cumError < error, n++,
cumError += N[Abs[Ctable[[degr
+ 1 - n]]]];
Null];
Stable = Drop[Ctable, -(n - 1)];
```

TABLE II
Near-Field Telescoped Coefficients, C_n , in Eq. (20) and Maximum Error for Truncation Order p

p= Error= n	4 9.0×10^{-4} C_n	6 6.0×10^{-5} C_n	7 1.5×10^{-5} C_n	9 9.0×10^{-7} C_n	11 6.0×10^{-8} C_n
0	+1.000168424170	+0.999989486047	+0.999989486047	+1.000000676740	+0.999999955579
1	-0.493294425973	-0.500576291916	-0.499952777942	-0.500003763858	-0.499999705374
2	+0.363417140132	+0.376300684829	+0.376300684829	+0.374868276727	+0.375012507912
3	-0.411484194544	-0.294974339461	-0.314926786620	-0.312207537771	-0.312532216473
4	+0.386263387620	+0.248838910848	+0.248838910848	+0.277487072894	+0.272871674970
5		-0.372831536266	-0.213211958996	-0.252369142421	-0.245096339495
6		+0.366465271393	+0.366465271393	+0.183117034297	+0.234809491040
7			-0.364844748048	-0.156006436446	-0.222500634623
8				+0.366696474192	+0.130388100512
9				-0.371268109514	-0.105291316807
10					+0.378093397888
11					-0.386875334847

```
Ttable = Table[ChebyshevT[i, x], {i,
0, degr + 1 - n}];
Return[Apart[Stable . Ttable]];
Null]
```

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