A Very Fast and Momentum-Conserving Tree Code

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ABSTRACT

The tree code for the approximate evaluation of gravitational forces is extended and substantially accelerated by including mutual cell-cell interactions. These are computed by a Taylor series in Cartesian coordinates and in a completely symmetric fashion, such that Newton’s third law is satisfied by construction and hence momentum exactly conserved. The computational effort is further reduced by exploiting the mutual symmetry of the interactions. For typical astrophysical problems with \(N=10^5\) and at the same level of accuracy, the new code is about four times faster than the tree code. For large \(N\), the computational costs are found to scale almost linearly with \(N\), which can also be supported by a theoretical argument, and the advantage over the tree code increases with ever larger \(N\).

Subject headings: methods: n-body simulations – methods: numerical – stellar dynamics

1. Introduction

The tree code (cf. Barnes & Hut 1986, hereafter B&H) has become an invaluable tool for the approximate but fast computation of the forces in studies of collisionless gravitational dynamics. It has been applied to a large variety of astrophysical problems. The gravitational potential generated by \(N\) bodies of masses \(\mu_n\) and at positions \(X_n\) is

\[
\Phi(X) = -\sum_{n=1}^{N} \mu_n g(|X - X_n|),
\]

(1)

where \(g(r)\) denotes the greens function, i.e. for unsoftened gravity \(g(r) = G/r\). The essence of the tree code is to approximate this sum over \(N\) terms by replacing any partial sum over all bodies within a single cell which is well-separated from \(X\) by just one term. The inner structure of the cell is partly taken into account using its multipole moments. This method reduces the overall costs for the computation of all forces from \(O(N^2)\) to \(O(N \log N)\).

The tree code, however, does not exploit the fact that the force due to the contents of some cell is very similar at nearby positions (even though one may use the fact that nearby bodies tend to have very similar interaction lists, cf. Barnes 1990). Exploiting this is the idea of the fast multipole method (FMM) (Greengard & Rokhlin 1987). The FMM employs a (usually) non-adaptive structure of hierarchical grids and considers only interactions between nodes on the same grid level according to their geometrical neighbourhood. The gravitational field due to some source cell and within some sink cell is approximated by a multipole expansion in spherical harmonics, the order of which is adapted to meet predefined accuracy limits. This method has been claimed to reduce the overall amount of operations to \(O(N)\), but the tables given by Cheng, Greengard & Rokhlin (1999) do not support this claim. Capuzzo-Dolcetta & Micocchi (1998) find that the FMM needs \(O(N \log N)\) operations, and is significantly slower for astrophysical applications than the tree code at comparable accuracy.

Instead of using a spherical multipole expansion of adaptive order, it is actually more efficient to use a Cartesian expansion of fixed order. Moreover, by preserving the symmetry of the gravitational interaction for mutual cell-cell interactions, one can (i) reduce the computational effort and (ii) obtain a code that satisfies Newton’s third law by construction and hence results in exact conservation of momentum, a property not shared by the traditional tree code.

2. Description of the Code

We start as the B&H tree code with a hierarchical tree of cubic cells. Each cell has up to eight sub-nodes cor-
responding to its octants. A node can be either a single body or another cell. The tree-building phase (cf. B&H) also includes the computation of the cells’ masses, centers \( Z \) of mass, and quadrupole moments.

### 2.1. The Opening Criterion

In order to benefit from the symmetry of the gravitational interaction, the opening criterion, which decides whether or not two nodes are well-separated so that a direct mutual interaction is acceptable, must be symmetric, too. We employ an extension of the criterion used in the tree-code: nodes A and B are well-separated if

\[
|Z_A - Z_B| > \left( r_{\text{max}A} + r_{\text{max}B} \right) / \theta, \tag{2}
\]

where the opening angle \( \theta \) controls the accuracy of the code. \( r_{\text{max}} \) is the radius of a sphere centered on the node’s center of mass and enclosing all bodies within it. Bodies naturally have \( r_{\text{max}} \equiv 0 \), i.e. two bodies are always well separated, while for the interaction between a body and a cell the criterion (2) reduces to that used in the tree code. Note that if one additionally to equation (2) requires \( r_{\text{max}A} = 0 \), the standard tree code is recovered, but the symmetry between A and B is broken.

There exist two upper limits for the radius \( r_{\text{max}} \). One is the distance \( b_{\text{max}} \) between the cell’s center of mass, \( Z \), and its most distant corner (Salmon & Warren 1994). The other is

\[
\max_{\text{sub-nodes} \ i} \left( r_{\text{max}i} + |Z_i - Z| \right) \tag{3}
\]

(Benz et al. 1990). After computation of both these upper limits, we take the smaller one to be \( r_{\text{max}} \). For cells with only a few bodies like cell A in Fig. 1, the latter often gives values significantly smaller than \( b_{\text{max}} \), while for cells with many bodies, like cell B in Fig. 1, \( b_{\text{max}} \) is the tighter limit.

### 2.2. Approximating Gravity

Consider two bodies at \( X \) and \( Y \) which reside in two well-separated cells A and B with centers of mass at, respectively, \( Z_A \) and \( Z_B \) and separation \( R = Z_A - Z_B \). We may re-write \( X - Y = R + (x - y) \) with \( x = X - Z_A \) and \( y = Y - Z_B \) being small in magnitude compared to \( R \) (because the cells are well-separated, cf. Fig. 1). The Taylor expansion of \( g(|X - Y|) \) around \( R \) reads

\[
g(|X - Y|) = \sum_{p} \frac{1}{p!} \left[ (x - y) \cdot \nabla \right]^p g(|r|) \bigg|_{r=R}. \tag{4}
\]

Separating powers of \( x \) from powers of \( y \) in equation (4) and subsequently taking the mass weighted sum over cell B yields a Cartesian multipole expansion of the potential \( \Phi_{B \rightarrow A}(X) \) at any position \( X \) within cell A and due to all bodies inside cell B (Warren & Salmon 1995). Since \( Z_B \) was chosen to be the center of mass of cell B, its dipole vanishes. The highest-order multipole occurring in such an expansion may actually be omitted, since it only contributes a constant to the approximation for \( g \) and does not affect the approximation for \( \nabla g \) and hence the force. The expression of third order thus reads (without the octopole; using Einstein’s sum convention)

\[
\Phi_{B \rightarrow A}(X) \approx M_B \left\{ \begin{array}{c}
D^{(0)} + \frac{1}{3} \tilde{Q}_{Bij} D^{(2)}_{ij} \\
+ x_i \left(D^{(1)}_i + \frac{1}{2} \tilde{Q}_{Bjk} D^{(3)}_{ijk}\right) \\
+ \frac{1}{2} x_i x_j D^{(2)}_{ij} + \frac{1}{6} x_i x_j x_k D^{(3)}_{ijk}\end{array} \right\}, \tag{5}
\]

where \( M_B \) and \( \tilde{Q}_{Bij} \) are the mass and specific quadrupole moment

\[
\tilde{Q}_{Bij} = \frac{1}{M_B} \sum_{y_n \in \text{cell B}} \mu_n y_n i y_n j \tag{6}
\]

of cell B, while \( D^{(n)} \equiv \nabla^n g(r) \big|_{r=|R|} \), i.e.

\[
\begin{aligned}
D^{(0)} &= D^0, \\
D^{(1)}_i &= R_i D^1, \\
D^{(2)}_{ij} &= \delta_{ij} D^1(R) + R_i R_j D^2, \\
D^{(3)}_{ijk} &= (\delta_{ij} R_k + \delta_{jk} R_i + \delta_{ki} R_j) D^2 + R_i R_j R_k D^3
\end{aligned} \tag{7}
\]

with

\[
D^n \equiv \left( \frac{1}{r} \frac{\partial}{\partial r} \right)^n g(r) \bigg|_{r=|R|}. \tag{8}
\]

The symmetry between \( x \) and \( y \) at every order of the Taylor expansion in equation (4) has two important consequences. First, if this expansion is used to compute
both $\Phi_{B \rightarrow A}(X)$ and $\Phi_{A \rightarrow B}(Y)$, Newton’s third law is satisfied by construction. Note, that our omission of the octopole term broke the symmetry only in the zeroth order and has no effect on the forces.

Second, the expressions for $M_A \Phi_{B \rightarrow A}$ and $M_B \Phi_{A \rightarrow B}$ are very similar: the expansion coefficients of second and third order differ only by mere signs, such that computing these coefficients for both Taylor series at one time is substantially faster than computing them at different times.

The transformation, or shifting, of the expansion center to some other position is trivial compared to the analogous procedure in the FMM (see Cheng et al.).

### 2.3. The Algorithm

The standard tree code computes the forces on each body by a recursive tree walk, which visits each node exactly once as a gravity sink, and thus exhibits an inherent asymmetry between sources and sinks. The new algorithm avoids this asymmetry.

First, in the interaction phase, the Taylor series coefficients are evaluated and accumulated in data fields associated with each node. This phase is based on the concept of **mutual interactions** (MIs), pairs of nodes, A and B, such that bodies in node A must receive forces from all bodies in node B, and vice versa. We start by the MI describing the root-root self-interaction, and process a given MI as follows. (1) A body self-interaction is ignored; (2) a cell self-interaction is split into the MIs between the sub-nodes\(^1\), and the process is continued on each of the new MIs; (3) a MI representing a well-separated pair of nodes is executed: the Taylor coefficients are computed and added to the nodes’ corresponding data fields; (4) finally, in any other case, the node with larger $r_{\text{max}}$ is split, and up to eight new MIs are created and processed.

Secondly, in the collection phase, the Taylor coefficients are passed down the tree: the expansion center is shifted to the center of mass of the currently active cell and the coefficients are accumulated. The Taylor expansion is evaluated at the position of any body and the values for potential and acceleration are added to its data fields (which may already contain contributions accumulated during the interaction phase).

### 3. Performance Tests

We tested the new algorithm and compared it with the tree code in three typical astrophysical situations: (1) a spherical Plummer model, representing a rather homogeneous stellar system, (2) a spherical Hernquist-model (1990) galaxy, and (3) a group of five such galaxies with various masses and scale radii. We generated $10^5$ random initial positions from each of these cases, truncating the density at 1000 scale radii, and evaluated the exact mutual forces at all positions and the approximate forces due to the tree code (up to quadrupole order) and the new code for opening angles $\theta$ between 0.2 and 1. We used an optimally chosen softening with the biweight softening kernel (see Dehnen 2000), but the results are insensitive to these settings. Both approximation methods have been coded by the author\(^2\) and use

\(^1\)In a cubic oct-tree, these are at most 36 independent sub-MIs.

\(^2\)At the same $\theta$, the tree code is twice as fast as a code publicly available from J. Barnes, mainly because the new opening criterion leads to fewer interactions. However, even at the same number of interactions, the author’s code was about 30% faster.
the same opening criterion (§2.1). In order to measure the accuracy of the approximated forces, we evaluated (cf. Capuzzo-Dolcetta & Miocchi 1998)

\[ \varepsilon_n = |a_n - a_{nP}| / a_{nP}^{PP}, \tag{9} \]

where \( a_n \) denotes the magnitude of the acceleration of the \( n \)th body due to either of the approximate methods and \( a_{nP}^{PP} \) that of the exact computation.

Figure 2 plots the CPU time needed for the force approximation on a Pentium III/500Mhz PC versus the mean relative error and that at the 99 percentile. For the new code, the time consumption scales almost inversely with the error, while the tree code flattens off\(^3\) at \( \theta \gtrsim 0.7 \). Evidently, at an acceptable level of accuracy, e.g. \( \varepsilon_{99\%} = 0.01 \), the new code is about four times faster than the tree code, even though it requires a smaller amount of CPU time per body. This can be explained as follows. Arranging eight root cells to a new root box, increases \( N \) to \( 8N \) and the number \( N_I \) of interactions to \( 8(N_I + N_r) \), where \( 8N_r \) interactions are needed to compute the forces between the former root cells. Thus,

\[ \frac{dN_I}{dN} \approx \frac{N_I \Delta \log N_I}{N \Delta \log N} = \frac{N_I + N_r / \ln 8}{N}. \tag{10} \]

In the tree code, \( N_r \propto N \) yielding \( N_I \propto N \log N \). In the new code, \( N_r \) may be estimated to contain two contributions, a constant term accounts for the interactions with distant nodes, and a term \( \propto N^{2/3} \) for those on the surface of the former root cells. Inserting this into equation (10) yields

\[ N_I \propto N - c_1 N^{2/3} - c_2 \tag{11} \]

with constants \( c_1 \) and \( c_2 \) that depend on \( \theta \). Thus, at large \( N \), a linear relation is approached. Note that this argument differs from that given for the FMM by Greengard & Rokhlin (1987), who assumed that the resolution may remain fixed when increasing \( N \).

\(^3\)This is, because of \( \tau_{\text{max}} \) is not proportional to the cell size, so that increasing \( \theta \) from 0.7 does not much decrease the number of interactions.

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**Figure 3.**— CPU time per body plotted versus \( N \) for test case 2 (Hernquist model)

4. Discussion

A new code for the approximate evaluation of gravitational forces has been presented, tested, and compared to the tree code. This new code is substantially faster than the tree code. Moreover, unlike the latter, it satisfies Newton’s third law by construction, such that any \( N \)-body code based on it will not introduce spurious net accelerations. The new code is based on a Taylor expansion of the Green’s function in Cartesian coordinates and incorporates mutual cell-cell interactions. The simple algorithm is well suited for implementation on parallel computers: different mutual interactions (MIs) can be passed to different CPUs.

The scaling of the CPU time required for the mutual forces of a number \( N \) of bodies becomes essentially linear at \( N \gtrsim 10^3 \), so that with ever larger \( N \) the new code is increasingly faster than the tree code, allowing for a substantial improvement in simulations employing large number of bodies. The only disadvantage is the increased requirement of memory compared to the standard tree code: 20 floating point numbers per cell are needed to hold the Taylor expansion coefficients. (By using a tree-walking algorithm instead of that given in §2.3, one can avoid this at the price of enhanced CPU time consumption.)

In spirit, the new code is similar to Greengard & Rokhlin’s (1987) fast multipole method, but is more efficient because it (i) uses a Cartesian instead of a spherical harmonic multipole expansion and (ii) fixes the order of the expansion while controlling the accuracy via the interaction condition, rather than fixing the interactions and adapting the expansion order to the accuracy.
A concern with codes based on cell-cell interactions is their performance in the presence of individual time steps. Clearly, when not all the forces are to be computed, such codes fare less favorably. However, when the forces for all bodies within some domain are desired, the new code is still a significant improvement over the tree code.

The new code has been written in C++ and will be electronically available from the author upon request.

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