Natively Periodic Fast Multipole Method: Approximating the Optimal Green’s Function

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Abstract

The fast multipole method (FMM) obeys periodic boundary conditions “natively” if it uses a periodic Green’s function for computing the multipole expansion in the interaction zone of each FMM oct-tree node. One can define the “optimal” Green’s function for such a method that results in the numerical solution that converges to the equivalent particle-mesh (PM) solution in the limit of sufficiently high order of multipoles. A discrete functional equation for the optimal Green’s function can be derived, but is not practically useful as methods for its solution are not known. Instead, this paper presents an approximation for the optimal Green’s function that is accurate to better than $10^{-3}$ in $L_{\text{MAX}}$ norm and $10^{-4}$ in $L_2$ norm for practically useful multipole counts. Such an approximately optimal Green’s function offers a practical way for implementing the FMM with periodic boundary conditions natively, without the need to compute lattice sums or to rely on hybrid FMM-PM approaches.

Unified Astronomy Thesaurus concepts: Computational methods (1965)

1. Introduction

Numerical simulations most commonly model a limited spatial volume, but actual space has no limits; hence, in many astrophysical applications numerical simulations have to employ periodic boundary conditions as a makeshift representation of unlimited space. Given an approximate representation of physical reality (discussing pros and cons of such an approximation is not a subject of this paper), one can then address a mathematically exact question of implementing periodic boundary conditions in a computational algorithm. For gravity calculations, imposing periodicity is not necessarily trivial. It is, of course, trivial for the simple particle-mesh (PM) method (Hockney & Eastwood 1988) that uses the discrete fast Fourier transform (FFT) to compute the gravitational potential (and/or accelerations) on the uniform grid. The discreteness of the FFT ensures that scales larger than the computational box size (i.e., waves with spatial frequencies below the fundamental frequency) do not contribute to the Green’s function $G$ that is used to compute the potential from the assigned density on the grid.

In modern simulations multipole-based methods are commonly used to compute the gravitational accelerations for particles or for cells on a grid, such as a classical Barnes–Hut method (Barnes & Hut 1986) or a fast multipole method (FMM) introduced by Greengard & Rokhlin (1987, 1997) and Cheng et al. (1999). In cosmological simulations the problem of imposing periodic boundary conditions for tree or FMM methods has been traditionally solved by using hybrid tree-PM and FMM-PM approaches, as implemented in, for example, the widely used cosmological code GADGET (Springel 2005; Springel et al. 2020). In such methods the gravitational force is split into a short-range part that is solved by a tree or an FMM and a long-range part that is solved on a uniform grid with a PM method. Because the two parts of the full gravitational force are solved with two different methods, an error is always introduced at scales where the two components are comparable. For example, in GADGET such an error can reach $\sim 1\%$ (Springel 2005; Springel et al. 2020). It is not presently known if that error results in simulation artifacts.

Since the FMM computes a convolution of the density distribution with a Green’s function, one can simply use a periodic Green’s function to compute the convolution with periodic boundary conditions, in a direct analogy to the PM method. Such an FMM method would have periodic boundary conditions “natively,” without any additional computations. This is, of course, not a new idea and has been proposed in the past (see Yan & Shelley 2018). A choice, however, needs to be made as to which Green’s function to use.

While in the continuous limit in 3D there is just one Green’s function for the gravitational potential,

$$G_0(x) = \frac{1}{4\pi r}$$

(or $\tilde{G}_0(k) = -1/k^2$ in Fourier space—hereafter I use a tilde symbol to label the Fourier transform of a function), this is not so for a discrete problem. In fact, on a uniform grid there are infinitely many Green’s functions that approach $G_0$ in the continuous limit. One such function is the “exact-in-Fourier-space” Green’s function,

$$\tilde{G}_k(k) = \begin{cases} -1/k^2, & k \neq 0 \\ 0, & k = 0 \end{cases}$$

which is the integer-valued vector on an $N^3$ grid, $n = (n_x, n_y, n_z)$ with

$$x = -N/2 + 1, -N/2 + 2, \ldots, -1, 0, 1, \ldots, N/2 - 1, N/2.$$  

Another extreme is the “exact-in-real-space” Green’s function,

$$G_{\chi}(x) = -\frac{1}{4\pi} g(|x \odot L|),$$

where $g(r) = 1/r$ in 3D and $g(r) = \log(r^2)$ in 2D and the symbol $\odot$ denotes the periodic coordinate wrap in a box of size $L$.
Examples of the exact-in-real- and the exact-in-Fourier-space Green’s functions in 2D in real space.

\[ x \oplus L = x - L \text{nint}(x/L), \]

where nint() is the function returning the nearest integer to a real number. A particular feature of \( G_X \) is that it is continuous but not differentiable at \(|x| = L/2\).

These two examples of Green’s functions for a 2D case are shown in Figure 1. One can construct infinitely many Green’s functions between these two extremes. For example, the Green’s function that enters the commonly used Ewald summation technique (Ewald 1921) is simply

\[
G_E(x) = G_X(x) \text{erfc}(r/\rho_s) + \frac{1}{2\pi^{3/2}\rho_s} \sum_{k} \left[ \hat{G}_K(k) e^{-|k|^2/4} \right]
\]

for some \( \rho_s \ll L \) (in which case additional terms due to periodic images are negligible). The Ewald summation Green’s function approaches \( G_X \) (up to a constant) for \( r \ll \rho_s \) and \( G_K \) for \( r \gg \rho_s \).

2. Natively Periodic FMM

The FMM algorithm uses an oct-tree (in 3D) to tessellate the space. In what follows I assume that the tree has at least three levels of refinement as the general case—special cases of shallower trees can be considered similarly. For levels above three no assumptions about the structure of the oct-tree need to be made, and the tree structure can be completely arbitrary as a three no assumptions about the structure of the oct-tree need to be made, and the tree structure can be completely arbitrary as a

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单FFT与PM方法类似。因此，唯一需要改变的是将HPM方法应用于具有原始周期性的FMM。所以，使用合适的Green函数对FFT进行积分。

3. Optimal Green’s Function

The choice of the “appropriate Green’s function” is not trivial, however. As an example, Figure 3 shows solutions for the gravitational potential by the PM and FMM-HPM methods with the exact-in-real-space Green’s function $G_X$ (Equation (2)). For this test the FMM-HPM method is implemented with the code described in Gnedin (2019). The oct-tree is at least three levels deep (with just two levels the PM and FMM-HPM results are identical by construction). Each FMM oct-tree node is covered by a 16² subgrid (for this 2D test, and by a 16³ subgrid for the 3D tests presented below) — the choice of the size of the subgrid is dictated by the requirement that it is significantly larger than the largest number of multipoles used in the tests below; otherwise there is an accidental cancellation of errors that misrepresents the real accuracy of the FMM. Thus, the total box is covered by the uniform $128^D$ grid ($D$ is the dimension of space), which is the grid used by the PM method. The gravitational source is modeled by assigning the density of $1/128^D$ in the lowest-left cell of the uniform grid, so that the total mass of the source is 1 if the box size is taken to be 1. A number of other, randomly chosen locations were tested, and the corner source was found to result in the largest error possible (i.e., it is the worst case scenario — this is also illustrated below).

The definition of the error between the PM and FMM-HPM methods also requires special consideration. In the PM method gravitational accelerations are computed from the potential by the 4th order finite difference (up to the 8th order was tested, the 4th order was found to give a converged answer), while in the FMM method the accelerations are computed from the multipole expansion. The difference between the accelerations from the FMM and from the PM method is made of these two contributions: (a) the error due to the choice of the Green’s function and (b) the error in the multipole expansion. In order to only compute (a), the error in the multipole expansion is estimated by comparing the FMM and PM method in the nonperiodic case. Hence, the error due to the choice of the Green’s function is computed as

$$\Delta g = |g_{FMM}^P - g_{PM}^P - (g_{FMM}^{NP} - g_{PM}^{NP})|,$$

where superscripts $P$ and $NP$ stand for “periodic” and “nonperiodic.” The error due to the multipole expansion is also shown below in Figure 5. Such a correction is not perfect, of course, hence the errors due to the choice of the Green’s function presented below may be somewhat overestimated.

Ideally, the relative error would be most informative. However, for a single source in a box with periodic boundary conditions there is a location where the gravitational acceleration vanishes identically and planes where each of the components of the acceleration vanishes. Hence, small absolute errors near such locations result in large relative errors. The search for the optimal Green’s function below utilizes minimization of some norm of the error. In order to avoid the error to be dominated by just one location in the computational box, the absolute error is used hereafter. In a unit box with $GM = 1$ the characteristic gravitational acceleration is 1, so the absolute error measures the relative error with respect to that characteristic acceleration.

The absolute error between the PM and FMM-HPM methods when both use the exact-in-space Green’s functions $G_X$ is shown in the right panel of Figure 3. That error is very large, primarily due to sharp features in the gravitational potential from the FMM-HPM method. These features arise from aliasing in the exact-in-real-space Green’s function $G_X$ since, as mentioned above, $G_X$ is not differentiable at the distance of half the box size.

While the two solutions are different, they both are valid solutions of the Poisson equation with periodic boundary conditions. Intuitively, however, it seems that the PM solution is in some sense “better.” While this is not a mathematically rigorous statement, I adopt it as an ansatz in the rest of this paper. One can then define an “optimal” Green’s function $G_a$ for the natively periodic FMM as the Green’s function with which the PM method and the FMM produce the same gravitational potential.

A reasonable question to ask is why the two Green’s functions should be the same. For example, one can use a PM method with the exact-in-Fourier-space Green’s function $G_X$ and then choose the Green’s function for the FMM such that the solutions agree. That would not be possible, however. For the solutions to match, the FMM solution in the near zone

Figure 3. Solutions in 2D for the gravitational potential from a point source located in the lower-left corner of the box with the exact-in-real-space Green’s function (Equation (2)) and $N_f = 6$ gridlet ($6^2$ Cartesian multipoles). The left panel shows the PM method, while the middle panel shows the FMM-HPM method. The right panel shows the difference in the gravitational acceleration between the two, which in the worst case exceeds 100% due to the catastrophic aliasing in the exact-in-real-space Green’s function $G_X$. 

...
should match too. For a regular grid, this can be solved with a PM-like method, using FFT with nonperiodic boundary conditions (which are most easily achieved by doubling the grid size—this is the approach taken in this paper). If the Green’s function used in the global PM solution does not match exactly the one used in the near zone part of the FMM computation, the two solutions would differ near the source, precisely where the force is the largest, resulting in a large absolute error even from small relative errors.

The requirement that the PM and the FMM solutions agree is not mathematically rigorous due to the existence of additional errors due to multipole expansion—a realistic realization of the FMM would never agree with the PM solution exactly because the FMM solution is (almost) always approximate. One can derive a mathematically rigorous result in the limit when the FMM uses Cartesian multipoles of the order equal to the size of the subgrid. In that special case, there is no error due to the multipole expansion in the interaction zone.

In order to derive the equation for the optimal Green’s function $G_a$, let us consider the three-level deep oct-tree. Given the distribution of masses $M_p$ on the gridlet in a level 3 node, the PM solution for the potential in some other oct-tree node is simply a convolution over that node gridlet (because in the special case considered the size of the gridlet is equal to the size of the subgrid in that oct-tree node),

$$\Phi^\text{PM} = \sum_q G_a(d + \Delta x(p - q)) M_q,$$

where $p$ and $q$ are vector-valued indices over the gridlets, $p = (p_x, p_y, p_z)$, $p = (p_x, p_y, p_z)$, $p_t = 0, \ldots, N_p - 1$, with $N_p$ being the gridlet size (6 in the test shown in Figure 3); $\Delta x = 1/(8N_p)$ is the gridlet spacing (the size of one cell on the PM mesh), and $d$ is the vector from the center of the source oct-tree node to the target oct-tree node.

The same computation in the FMM-HPM method would take three steps:

1. projecting the source multipoles from a child node $C_s$ at level 3 ($M_q^{L=3}$) to level 2 ($M_q^{L=2}$),

$$M_q^{L=2} = \sum_q T^{C_s}_{L=2} M_q^{L=3},$$

where matrices $T_{L=2}$ are defined in Section 2.3 of Gnedin (2019);

2. computing the interaction zone contribution to the multipoles on level 2,

$$\Phi_{r}^{L=2} = \sum_s G_a(d_{L=2} + \Delta x_{L=2}(r - s)) M_q^{L=2},$$

and

3. projecting the level 2 multipoles up to a child node $C_T$ at level 3,

$$\Phi_{p}^{L=3} = \sum_r T^{C_T}_{L=3} \Phi_{r}^{L=2}.$$

Comparing Equation (4) with Equations (5)–(7) and requiring that $\Phi^\text{PM} = \Phi^\text{FMM}$ plus const for any $M_q$, one arrives at the equation on $G_a$:

$$G_a(d + \Delta x_{L=3}(p - q)) = \text{const} + \sum_{r,s} T^{C_T}_{r} T^{C_T}_{rs} G_a(d_{L=3} + \Delta x_{L=3}(r - s)).$$

Since $\Delta x_{L=2} = 2\Delta x_{L=3}$ for an oct-tree and the source and target child nodes are offset from their respective parent node centers by vectors $a^C_T$ and $a^C_T$, one can rewrite the equation for $G_a$ as

$$G_a(d + a^C_T - a^C_T + \Delta x(p - q)) = \text{const} + \sum_{r,s} T^{C_T}_{rs} G_a(d + 2\Delta x(r - s)), (8)$$

with $\Delta x$ being the size of the cell on the PM mesh. Notice that $G_a$ may be a function of the gridlet size $N_p$ (or, equivalently, the number of multipoles $N^3$) since for different gridlet sizes Equation (8) is different.

The challenge of solving Equation (8) is twofold: first, it is a discrete functional equation and does not belong to any class of mathematical equations for which methods of solution are known. Second, the vector $d$ is well known, the vector $d$ from one oct-tree node center at level 2 to another oct-tree node in the first node interaction zone, i.e., Equation (8) does not constrain $G_a(d)$ everywhere in space but only for $x$ such that at least one of its components is greater than $L/4$ by absolute value (the latter is not a serious limitation if $G_a$ is assumed to be analytic).

In trying to solve Equation (8), I attempted to use several simple iteration schemes, but found none that converged. An alternative approach to finding an approximation to the optimal Green’s function is to assume a parameterized functional form for $G_a$ and fit for the best parameter values.

In the following, I adopt the following ansatz:

$$G_a(x) \approx G_a(x) = -\frac{1}{4\pi} \theta(|\hat{x} \cdot L|),$$

where $\hat{x}$ should approach $x$ at small scales to recover the Newtonian force and should be differentiable at half the box size to avoid catastrophic aliasing from Figure 3. One such choice for $\hat{x}$ is

$$\hat{x} = L \xi_n \left( \frac{x}{L} \right),$$

with

$$\xi_n(t) = \sin(\pi t) + \sum_{k=1}^n \alpha_k \sin((2k + 1) \pi t) \frac{\sin((2k + 1) \pi t) - \sin(\pi t)}{\pi}.$$
complexity. Why this is so is clear from Figure 4, which shows the error in the acceleration for the “approximately optimal” Green’s function $G_S$ with $n = 1$ and the value of the coefficient $a_1$ (as well as the accuracy of the fit) given in Table 1. The error is reduced by almost three orders of magnitude compared to the worst case. In all tests considered the Green’s function error is below or about the error due to the multipole expansion for $N_S < 10$. For the 10 random source test the error due to the approximate Green’s function is similar to the error due to the multipole expansion, indicating that the subtraction of the multipole expansion error in Equation (3) is inaccurate for that test. For practical numbers of multipoles ($N_S > 6$—for example, $N_S = 8$ in the ABACUS code Garrison et al. 2019) the Green’s function error is below $L_{MAX} = 10^{-3}$ or $L_2 = 10^{-5}$, which is significantly smaller than the similar error in the tree-PM approach (Springel et al. 2020).

Figure 6 shows the deviations of the FMM gravitational acceleration computed using the $G_S$, Green’s function from the exactly Newtonian form. A similar comparison for the tree-PM method is presented in Springel et al. (2020). Deviations from the Newtonian form are not perfectly radial as in tree-PM, but generally significantly smaller.

### 4. Conclusions

The Green’s function

\[ G_{S1}(x) \equiv \frac{1}{4\pi} \delta(|\hat{\mathbf{x}} \cdot \mathbf{L}|), \tag{9} \]

with

\[ \hat{\mathbf{x}} = \frac{9L}{8\pi} \sin(\pi x / L) - \frac{L}{24\pi} \sin(3\pi x / L) \]

is an approximately optimal Green’s function for an implementation of the FMM algorithm that supports periodic boundary conditions natively, without computing lattice sums or relying on hybrid approaches like the FMM-PM method.

Where would one go from here? For many practical applications $G_{S1}$ would be enough as it is already more than 100 times more accurate in the $L_2$ sense and 20 times more accurate in the $L_{MAX}$ sense than the GADGET-4 tree-PM or FMM-PM approach (Springel et al. 2020, Figure 18). However, its primary limitation is that there is no clear path to improving its precision. I have also tried several other functional forms for $G_{\ast}$, including Taylor expansion of $G_{\ast}$ in powers of $\sin(fx)$ with $f$ as another parameter, but found none that improves upon $G_{S1}$ in any significant way. It does not mean that the improvement is not possible, of course, just that the correct functional form for $G_{\ast}$ has not been found yet.
One can imagine alternative approaches to higher precision. All minimization done in this paper relies on standard local minimum finders. Methods for searching beyond the local minimum, such as simulated annealing, may produce better results. Another possible approach is to parameterize $G_s$ with a very large number of parameters—for example, as a grid of values with every value being its own parameter. Minimizing such an extremely large dimensional problem is difficult, but is likely to lead to much higher precision. For example, in the FMM-HPM algorithm the Green’s function only needs to be sampled on the $(4N_g)^D$ grid, and for a realistic number of multipoles $N_g = 8$ in 3D this is $32^3 = 32,768$ values, a large minimization problem but certainly not beyond modern capabilities. With the grid model for $G_s$ it should be possible to find $G_s$ exactly, i.e., with zero error. As a final note, Figure 5 has an interesting feature—the error due to the periodic Green’s function continues to fall as the number of multipoles increases. Since $G_{31}$ is approximate, one would expect the error to saturate for sufficiently large $N_g$, reflecting the imperfect accuracy of $G_{31}$. This is not the case, however. One can hypothesize that, perhaps, $G_{31}$ is then the true limit of $G_s$ for $N_g \to \infty$. Unfortunately, it is not possible to test such a hypothesis without a method for solving Equation (8).

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