

Error and symmetry analysis of Misner's algorithm for spherical harmonic decomposition on a cubic grid

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Abstract

In an earlier paper, Misner (2004, *Class. Quant. Grav.*, 21, S243) presented a novel algorithm for computing the spherical harmonic components of data represented on a cubic grid. I extend Misner's original analysis by making detailed error estimates of the numerical errors accrued by the algorithm, by using symmetry arguments to suggest a more efficient implementation scheme, and by explaining how the algorithm can be applied efficiently on data with explicit reflection symmetries.

Key words: spherical harmonics, numerical simulation, spin-weighted spherical harmonics, fixed mesh refinement

1 Introduction

Spherical harmonic analysis of data is a common procedure in many applications in science and engineering. In numerical calculations structured on a cubic grid, however, extracting spherical harmonic components can be non-trivial since the spherical harmonic components Φ_{lm} of a function Φ are defined by integrals over spheres

$$\Phi_{lm}(t, r) = \oint \bar{Y}_{lm}(\theta, \phi) \Phi(t, r, \theta, \phi) d^2\Omega. \quad (1)$$

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(8). For a finite volume, this weighing scheme provides an approximation that scales as $\mathcal{O}(h)$, but, for a region that is also scaling with h , the resulting integral scales as $\mathcal{O}(h^2)$. This provides additional motivation for choosing $\Delta \propto h$ since most applications will require at least second order accuracy.

For higher than second order accuracy, a new scheme for computing the volume integrals is needed, but the rest of the analysis here holds true. Given such a scheme, the analysis here shows how to choose the remaining parameters to ensure that numerical errors scale like any desired power of the grid spacing.

4 Choosing the parameters

In practice, the grid spacing parameter h is usually chosen to resolve the sources without exceeding the physical limits of the computer. I would not expect, in general, that the grid spacing would be chosen based on the needs of this algorithm. For that reason, let me assume now that h is chosen, and discuss how to choose the remaining parameters N and Δ . In this section I will discuss some of the theoretical issues that should be considered when choosing the parameters, leading to a rule of thumb that is valid based on this analysis and my experience with the algorithm.

The error analysis of Section 3 implies that for fixed Δ , increasing the value of N decreases the error term. It also implies that for fixed N , increasing the value of Δ increases the error term. This suggests taking Δ as small as possible, and N as large as possible to make the error term as small as possible. This must be balanced, however, against practical limitations. Certainly the shell thickness Δ needs to be large enough so that there are some grid points within the shell, otherwise the whole procedure is undefined. For fixed N , a stronger restriction requires that the Legendre polynomial P_N can be resolved over the shell. Without this condition, there would seem to be no benefit to taking higher values of N . Getting higher accuracy in practice requires finding a proper balance between choosing Δ small and N large.

In making this balance, however, one must keep in mind that the error in the method is partially determined by the weighting scheme (8), which is only second order accurate in the grid spacing. I am, in addition, going to choose $\Delta \propto h$ for reasons described above. This already suggests that taking N larger than two is pointless, since choosing $N = 2$ already makes the piece of the error that is proportional to Δ scale like $\mathcal{O}(\Delta^4)$ (cf. Table 1), meaning that it will be an error term of sub-leading order in grid spacing. But once this term is of sub-leading order, it is much less important how large I choose Δ , provided that I still choose it proportional to the grid spacing. I therefore adopt the following

Rule of Thumb: Choose N just large enough to ensure that the error term proportional to Δ is an error term of sub-leading order in grid spacing. Choose Δ just large enough to safely resolve P_N on the shell.

With this rule of thumb, and the second order accurate weighting scheme (8), I found the choices $N = 2$ and $\Delta = 3h/4$ completely satisfactory for a second order accurate code. Note that this corresponds to Misner's choice of Δ in Ref. [1]. With $N = 2$ I found that larger values of Δ are also acceptable. Numerical results justifying these estimates appear in Ref. [2].

5 Symmetry issues

There are two points of interest related to this method of spherical harmonic decomposition and symmetries. The first was mentioned briefly in Section 2, namely that symmetry causes the metric G_{AB} to be real and sparse. The second deals with implementing the method for grids in which explicit symmetries are enforced on grid functions in order to reduce the computational load of the simulation. In these cases, in which data is not evolved over a whole extraction sphere, additional analysis is required to demonstrate that the method is well defined and to understand how to most efficiently implement it. The primary result on this second topic is that the adjoint harmonics Y^A of (11) have the same symmetries under reflection as the original spherical harmonics Y_A .

Consider first the implications of symmetry on the metric G_{AB} . The symmetries of the spherical harmonics, summarized in Table 2, cause the imaginary part of all terms in the integral (9) to cancel in pairs of points on the sphere related by reflections through coordinate planes. The reason is that each of the four signs $(+1, (-1)^m, (-1)^l, \text{ and } (-1)^{l+m})$ appears twice in Table 2, once for a term that is complex conjugated and once for a term that is not. The matrix is also sparse. By similar reasoning, for certain values of l and m , the terms in the integral (9) can cancel in sets of four. Both of these facts can be seen at once through a simple calculation. The idea is to break the integral into parts using the second and third columns of Table 2, and then to simplify using the last two columns. Considering first just the symmetries under reflection through the xy -plane and recalling the definition (9),

Planes	θ	ϕ	Sign	Conjugate
None	θ	ϕ	+1	no
x	θ	$\pi - \phi$	$(-1)^m$	yes
y	θ	$-\phi$	+1	yes
z	$\pi - \theta$	ϕ	$(-1)^{l+m}$	no
xy	θ	$\pi + \phi$	$(-1)^m$	no
xz	$\pi - \theta$	$\pi - \phi$	$(-1)^l$	yes
yz	$\pi - \theta$	$-\phi$	$(-1)^{l+m}$	yes
xyz	$\pi - \theta$	$\pi + \phi$	$(-1)^l$	no

Table 2

The table shows how the arguments of spherical harmonics transform under reflections through various Cartesian planes. The first column indicates which coordinates have their signs inverted, while the second and third columns give the new angular arguments to the spherical harmonic Y_{lm} . Alternatively, the fourth and fifth column show, respectively, the overall sign in front of and whether or not to complex conjugate the given spherical harmonic with the original angular arguments. The second row, for example, says that $Y_{lm}(-x, y, z) = Y_{lm}(\theta, \pi - \phi) = (-1)^m \bar{Y}_{lm}(\theta, \phi)$, where (θ, ϕ) are the angular coordinates of the point (x, y, z) . Note that this table differs slightly from that in Ref. [2]. The table here is correct.

$$G_{AB} = \oint \bar{Y}_{l_1 m_1}(\theta, \phi) Y_{l_2 m_2}(\theta, \phi) d^2 \Omega \quad (16a)$$

$$= \int_0^{2\pi} \int_0^{\pi/2} \bar{Y}_{l_1 m_1}(\theta, \phi) Y_{l_2 m_2}(\theta, \phi) d^2 \Omega \\ + \int_0^{2\pi} \int_0^{\pi/2} \bar{Y}_{l_1 m_1}(\pi - \theta, \phi) Y_{l_2 m_2}(\pi - \theta, \phi) d^2 \Omega \quad (16b)$$

$$= [1 + (-1)^{l_1+l_2}] \int_0^{2\pi} \int_0^{\pi/2} \bar{Y}_{l_1 m_1}(\theta, \phi) Y_{l_2 m_2}(\theta, \phi) d^2 \Omega. \quad (16c)$$

(I have suppressed the radial functions since they play no role here.) Repeating the procedure for reflections through the xz - and yz -planes shows that

$$G_{AB} = 2\sigma_{m_1+m_2, l_1+l_2} \int_0^{\pi/2} \int_0^{\pi/2} \text{Re} \left\{ \bar{Y}_{l_1 m_1}(\theta, \phi) Y_{l_2 m_2}(\theta, \phi) \right\} d^2 \Omega \quad (17)$$

where

$$\sigma_{m_1+m_2, l_1+l_2} \equiv 1 + (-1)^{m_1+m_2} + (-1)^{l_1+l_2} + (-1)^{m_1+m_2+l_1+l_2}. \quad (18)$$

This proves that the matrix is real. In addition, the matrix element is zero by symmetry whenever

$$\sigma_{m_1+m_2, l_1+l_2} = 0 \quad (19)$$

which is true for 56 of the 81 matrix elements that exist when considering a fixed value of n and all values of l and m for $l \leq 2$. Of the remaining

$m_1 + m_2$	$l_1 + l_2$	Number	Satisfies (19)
even	even	25	no
even	odd	16	yes
odd	even	20	yes
odd	odd	20	yes

Table 3

The table summarizes which entries of G_{AB} identically vanish because of the symmetries of the spherical harmonics under reflections through coordinate planes for all values of l and m with $l \leq 2$. (This is governed by equation (19).) Of the 81 possible matrix elements, only 25 have non-trivial values.

25 matrix elements, 9, of course, are the diagonal elements that go to unity in the continuum limit. The exact break-down of which such elements must be zero by symmetry is summarized in Table 3. Knowing that the matrix is real-symmetric and sparse allows for a more efficient implementation of the algorithm in general. It is also extremely useful in analyzing the algorithm in the context of the second topic of this section, explicit grid symmetries.

When evolving initial data with known symmetries, it is very common to evolve only that part of the data that is unique. In such cases, an appropriate symmetry boundary condition is applied at some edges of the grid. This is, however, inconvenient for wave extraction since computing spherical harmonic components (by any method) requires integrating over the full sphere. If data with octant symmetry, for example, is evolved only in a single octant, it is neither sufficient to apply the decomposition algorithm in that one octant nor to multiply the result of a single octant by 8 since the symmetry may forbid some modes as well as repeating them.

In principle the problem appears to be even more difficult for this particular decomposition method. Although the spherical harmonics have well defined symmetries under reflections, as summarized in Table 2, it is the adjoint harmonics that appear in (11). The adjoint harmonics, however, are constructed by contracting G^{AB} with the usual spherical harmonics, and this appears to mix different values of l and m . While this mixing does occur, the the matrix G_{AB} is sparse in just the right way to ensure that the adjoint harmonics have the same symmetries at the usual spherical harmonics.

A particular choice of the mapping $(n, l, m) \mapsto A$ makes this easiest to see. Specifically, considering all values of l and m with $l \leq 2$, there is a basis in

which G_{AB} takes block diagonal form

$$(G_{AB}) = \begin{pmatrix} \Xi_1 & & & \\ & \Xi_2 & & \\ & & \Xi_3 & \\ & & & \Xi_4 \end{pmatrix} \quad (20)$$

with all unwritten entries identically zero by symmetry. In this expression Ξ_1 is a $4N \times 4N$ matrix over the basis functions $B_1 = \{Y_{n00}, Y_{n2,-2}, Y_{n20}, Y_{n22}\}$; Ξ_2 is an $N \times N$ matrix over the basis functions $B_2 = \{Y_{n10}\}$; Ξ_3 is a $2N \times 2N$ matrix over the basis functions $B_3 = \{Y_{n1,-1}, Y_{n11}\}$; and Ξ_4 is a $2N \times 2N$ matrix over the basis functions $B_4 = \{Y_{n2,-1}, Y_{n21}\}$. In this basis the matrix is block diagonal, so the inverse matrix

$$(G^{AB}) = \begin{pmatrix} \Xi_1^{-1} & & & \\ & \Xi_2^{-1} & & \\ & & \Xi_3^{-1} & \\ & & & \Xi_4^{-1} \end{pmatrix} \quad (21)$$

is also block diagonal and *the different basis sectors do not mix*. This last point is key. It implies that any particular adjoint harmonic is a linear combination of spherical harmonics from a single set B_k

$$Y^{nlm} = \sum_{Y_{n'l'm'} \in B_k} (\Xi_k)^{(nlm)(n'l'm')} Y_{n'l'm'} \quad (22)$$

where k is the index such that $Y_{nlm} \in B_k$. Because, in each set B_k , the parity of l and the parity of m is the same on each $Y_{nlm} \in B_k$, and because, in light of Table 2, it is the parity of l and m that determines the symmetries of Y_{nlm} under reflections through planes, every spherical harmonic in B_k for any fixed k has the same symmetries under reflections as any other spherical harmonic in B_k . This implies that the adjoint harmonics also share this symmetry under reflection.

6 Discussion

In this paper I have provided detailed error estimates of the Misner algorithm for computing spherical harmonic components of data represented on a cubic grid. This analysis allows one, in principle, to chose the parameters of the algorithm such that its numerical errors scale any desired power of the grid

spacing. The only limitation of this in practice is finding a scheme for approximating volume integrals on a shell of sufficiently high accuracy. (Misner's original choice allows for a second order accurate result.)

In addition, analysis of the symmetry properties of the spherical harmonics provides two insights: First, the number of operations required to initialize the data structures used to compute spherical harmonic components can be reduced by computing only those elements of G_{AB} that are not forbidden by symmetries, and, second, that the adjoint harmonics used by the algorithm have the same symmetries under reflections as the usual spherical harmonics. This second fact allows the method to be efficiently used on data with explicit grid symmetries when only the independent portion of that data is evolved.

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