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Short Note

# Fast algorithms for spherical harmonic expansions, III

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ABSTRACT

We accelerate the computation of spherical harmonic transforms, using what is known as the butterfly scheme. This provides a convenient alternative to the approach taken in the second paper from this series on "Fast algorithms for spherical harmonic expansions". The requisite precomputations become manageable when organized as a "depth-first traversal" of the program's control-flow graph, rather than as the perhaps more natural "breadth-first traversal" that processes one-by-one each level of the multilevel procedure. We illustrate the results via several numerical examples.



## 1. Introduction

The butterfly algorithm, introduced in [10,11], is a procedure for rapidly applying certain matrices to arbitrary vectors. (Section 3 below provides a brief introduction to the butterfly.) The present paper uses the butterfly method in order to accelerate spherical harmonic transforms. The butterfly procedure does not require the use of extended-precision arithmetic in order to attain accuracy very close to the machine precision, not even in its precomputations — unlike the alternative approach taken in the predecessor [15] of the present paper.

Unlike some previous works on the butterfly, the present article does not use on-the-fly evaluation of individual entries of the matrices whose applications to vectors are being accelerated. Instead, we require only efficient evaluation of full columns of the matrices, in order to make the precomputations affordable. Furthermore, efficient evaluation of full columns enables the acceleration of the application to vectors of both the matrices and their transposes. On-the-fly evaluation of columns of the matrices associated with spherical harmonic transforms is available via the three-term recurrence relations satisfied by associated Legendre functions (see, for example, Section 5 below).

The precomputations for the butterfly become affordable when organized as a "depth-first traversal" of the program's control-flow graph, rather than as the perhaps more natural "breadth-first traversal" that processes one-by-one each level of the multilevel butterfly procedure (see Section 4 below).

The present article is supposed to complement [11,15], combining ideas from both. Although the present paper is self-contained in principle, we strongly encourage the reader to begin with [11,15]. The original is [10]. Major recent developments are in [4,17]. The introduction in [15] summarizes most prior work on computing fast spherical harmonic transforms; a new application appears in [12]. These articles and their references highlight the computational use of spherical harmonic transforms in meteorology and quantum chemistry. The structure of the remainder of the present article is as follows: Section 2 reviews elementary facts about spherical harmonic transforms. Section 3 describes basic tools from previous works.

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Section 4 organizes the preprocessing for the butterfly to make memory requirements affordable. Section 5 outlines the application of the butterfly scheme to the computation of spherical harmonic transforms. Section 6 describes the results of several numerical tests. Section 7 draws some conclusions.

Throughout, we abbreviate "interpolative decomposition" to "ID" (see Section 3.1 for a description of the ID). The butterfly procedures formulated in [10,11] and the present paper all use the ID for efficiency.

## 2. An overview of spherical harmonic transforms

The spherical harmonic expansion of a bandlimited function $f$ on the surface of the sphere has the form

$$f(\theta,\varphi)=\sum_{k=0}^{2l-1}\sum_{m=-k}^{k}\beta_k^m\overline{P}_k^{|m|}(\cos(\theta))e^{im\varphi}, \tag{1}$$

where $(\theta,\varphi)$ are the standard spherical coordinates on the two-dimensional surface of the unit sphere in $\mathbb{R}^3$, $\theta\in(0,\pi)$ and $\varphi\in(0,2\pi)$, and $\overline{P}_k^{|m|}$ is the normalized associated Legendre function of degree $k$ and order $|m|$ (see, for example, Section 3.3 for the definition of normalized associated Legendre functions). Please note that the superscript $m$ in $\beta_k^m$ denotes an index, rather than a power. "Normalized" refers to the fact that the normalized associated Legendre functions of a fixed order are orthonormal on $(-1,1)$ with respect to the standard inner product. Obviously, the expansion (1) contains $4l^2$ terms. The complexity of the function $f$ determines $l$.

In many areas of scientific computing, particularly those using spectral methods for the numerical solution of partial differential equations, we need to evaluate the coefficients $\beta_k^m$ in an expansion of the form (1) for a function $f$ given by a table of its values at a collection of appropriately chosen nodes on the two-dimensional surface of the unit sphere. Conversely, given the coefficients $\beta_k^m$ in (1), we often need to evaluate $f$ at a collection of points on the surface of the sphere. The former is known as the forward spherical harmonic transform, and the latter is known as the inverse spherical harmonic transform. A standard discretization of the surface of the sphere is the "tensor product", consisting of all pairs of the form $(\theta_k,\varphi_j)$, with $\cos(\theta_0),\cos(\theta_1),\ldots,\cos(\theta_{2l-2}),\cos(\theta_{2l-1})$ being the Gauss–Legendre quadrature nodes of degree $2l$, that is,

$$-1<\cos(\theta_0)<\cos(\theta_1)<\ldots<\cos(\theta_{2l-2})<\cos(\theta_{2l-1})<1 \tag{2}$$

and

$$\overline{P}_{2l}^0(\cos(\theta_k))=0 \tag{3}$$

for $k=0,1,\ldots,2l-2,2l-1$, and with $\varphi_0,\varphi_1,\ldots,\varphi_{4l-3},\varphi_{4l-2}$ being equispaced on the interval $(0,2\pi)$, that is,

$$\varphi_j=\frac{2\pi(j+\frac{1}{2})}{4l-1} \tag{4}$$

for $j=0,1,\ldots,4l-3,4l-2$. This leads immediately to numerical schemes for both the forward and inverse spherical harmonic transforms whose costs are proportional to $l^3$.

Indeed, given a function $f$ defined on the two-dimensional surface of the unit sphere by (1), we can rewrite (1) in the form

$$f(\theta,\varphi)=\sum_{m=-2l+1}^{2l-1}e^{im\varphi}\sum_{k=|m|}^{2l-1}\beta_k^m\overline{P}_k^{|m|}(\cos(\theta)). \tag{5}$$

For a fixed value of $\theta$, each of the sums over $k$ in (5) contains no more than $2l$ terms, and there are $4l-1$ such sums (one for each value of $m$); since the inverse spherical harmonic transform involves $2l$ values $\theta_0,\theta_1,\ldots,\theta_{2l-2},\theta_{2l-1}$, the cost of evaluating all sums over $k$ in (5) is proportional to $l^3$. Once all sums over $k$ have been evaluated, each sum over $m$ may be evaluated for a cost proportional to $l$ (since each of them contains $4l-1$ terms), and there are $(2l)(4l-1)$ such sums to be evaluated (one for each pair $(\theta_k,\varphi_j)$), leading to costs proportional to $l^3$ for the evaluation of all sums over $m$ in (5). The cost of the evaluation of the whole inverse spherical harmonic transform (in the form (5)) is the sum of the costs for the sums over $k$ and the sums over $m$, and is also proportional to $l^3$; a virtually identical calculation shows that the cost of evaluating of the forward spherical harmonic transform is also proportional to $l^3$.

A trivial modification of the scheme described in the preceding paragraph uses the fast Fourier transform (FFT) to evaluate the sums over $m$ in (5), approximately halving the operation count of the entire procedure. Several other careful considerations (see, for example, [2,13]) are able to reduce the costs by 50% or so, but there is no simple trick for reducing the costs of the whole spherical harmonic transform (either forward or inverse) below $l^3$. The present paper presents faster (albeit more complicated) algorithms for both forward and inverse spherical harmonic transforms. Specifically, the present article provides a fast algorithm for evaluating a sum over $k$ in (5) at $\theta=\theta_0,\theta_1,\ldots,\theta_{2l-2},\theta_{2l-1}$, given the coefficients $\beta_{|m|}^m,\beta_{|m|+1}^m,\ldots,\beta_{2l-2}^m,\beta_{2l-1}^m$, for a fixed $m$. Moreover, the present paper provides a fast algorithm for the inverse procedure of determining the coefficients $\beta_{|m|}^m,\beta_{|m|+1}^m,\ldots,\beta_{2l-2}^m,\beta_{2l-1}^m$ from the values of a sum over $k$ in (5) at $\theta=\theta_0,\theta_1,\ldots,\theta_{2l-2},\theta_{2l-1}$. FFTs or fast discrete sine and cosine transforms can be used to handle the sums over $m$ in (5) efficiently. See [12] for a detailed summary and novel application of the overall method. The present article modifies portions of the method of [12,15], focusing exclusively on the modifications.