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Short Note

A fast and stable method for rotating spherical harmonic expansions

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ABSTRACT

In this paper, we present a simple and efficient method for rotating a spherical harmonic expansion. This is a well-studied problem, arising in classical scattering theory, quantum mechanics and numerical analysis, usually addressed through the explicit construction of the Wigner rotation matrices. We show that rotation can be carried out easily and stably through "pseudospectral" projection, without ever constructing the matrix entries themselves. Existing fast algorithms, based on recurrence relations, are subject to a variety of instabilities, limiting the effectiveness of the approach for expansions of high degree.

1. Introduction

Spherical harmonics arise in a variety of problems in mathematical physics. They can be viewed, for example, as the angular part of the separation of variables solution of the Laplace or Helmholtz equation in spherical coordinates or as the basis for Fourier analysis on the sphere. Taking the former perspective (briefly), we recall that any harmonic function u can be represented in spherical coordinates (r, θ, ϕ) as

$$u(r,\theta,\phi) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \left(L_n^m r^n + \frac{M_n^m}{r^{n+1}} \right) Y_n^m(\theta,\phi), \tag{1}$$

where

$$Y_n^m(\theta,\phi) \equiv \sqrt{\frac{2n+1}{4\pi}} \sqrt{\frac{(n-|m|)!}{(n+|m|)!}} \cdot P_n^{|m|}(\cos\theta) e^{im\phi}. \tag{2}$$

Here, ϕ is the azimuthal angle of the target point with respect to the x-axis and θ is the polar angle with respect to the z-axis. The Y_n^m are called spherical harmonics of degree n and order m. The special functions P_n^m are the associated Legendre functions and can be defined by the Rodrigues' formula

$$P_n^m(x) = (-1)^m (1-x^2)^{m/2} \frac{d^m}{dx^m} P_n(x),$$

where $P_n(x)$ is the usual Legendre polynomial of degree n [12,1,15].

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For functions regular at the origin, the coefficients M_n^m must be zero, while for functions regular at infinity, the coefficients L_n^m must be zero. The coefficients L_n^m and M_n^m are known as the moments of the expansion.

In the present paper, we are interested in the problem of expanding u in a rotated coordinate system. This arises as a computational task in quantum mechanics [1,7,15], scattering theory [13] and numerical analysis, particularly in some implementations of the fast multipole method (FMM) [4,8,9,17]. Since it is the angular coordinates (θ,ϕ) that are relevant, we may (without loss of generality) consider only functions on the unit sphere of the form

$$u(\theta,\phi) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} M_n^m Y_n^m(\theta,\phi). \tag{3}$$

1.1. Rotation operators

Let $\mathbf{E}$ denote the usual coordinate system defined by the axes:

$$e_1 = (1,0,0), \quad e_2 = (0,1,0), \quad e_3 = (0,0,1), \tag{4}$$

and let $\mathbf{F}$ be a rotated orthogonal coordinate system with the same origin and axes f_1, f_2, f_3. We will occasionally refer to P_E as the coordinate representation of a point P with respect to E and P_F as the coordinate representation of P with respect to F.

We assume that (α,β,γ) are the standard Euler angles [1,15] that define the rotation from $\mathbf{E}$ to $\mathbf{F}$ using the z—y—z convention in a right-handed frame. That is, we first rotate by an angle α about the z-axis, then by an angle β about the new y-axis, and finally by an angle γ about the new z-axis.

Theorem 1 (See, for example, [1]). *Let (θ,ϕ) denote the coordinates of a point P in the system $\mathbf{E}$ and let (θ',ϕ') denote the coordinates of P in the system $\mathbf{F}$. Then the function $u(P)$ defined in (3) can be expressed as*

$$u(\theta',\phi') = \sum_{n=0}^{\infty} \sum_{m'=-n}^{n} M_n^{m'} Y_n^{m'}(\theta',\phi'), \tag{5}$$

where

$$M_n^{m'} = \sum_{m=-n}^{n} D_n^{m',m} \cdot M_n^m. \tag{6}$$

The coefficients of the transformation are given by

$$D_n^{m',m} = e^{im\gamma} d_n^{m',m}(\beta) e^{im\alpha}, \tag{7}$$

where

$$d_n^{m',m}(\beta) = (-1)^{m'-m}[(n+m')!(n-m')!(n+m)!(n-m)!]^{1/2} r \sum_s (-1)^s \frac{(\cos\frac{\beta}{2})^{2(n-s)+m-m'} (\sin\frac{\beta}{2})^{2s-m+m'}}{(n+m-s)!s!(m'-m+s)!(n-m'-s)!}, \tag{8}$$

with the range of s determined by the condition that all factorials are non-negative.

Remark 1.1. The formula (8) is due to Wigner [18]. Note that the rotation operator uncouples spherical harmonics of different degree.

Suppose now that we have truncated the spherical harmonic expansion (3) at degree $n = p$, leaving $O(p^2)$ coefficients to consider. It is clear that the angle α and γ rotations about the z-axes in (7) are diagonal and require only $O(p^2)$ work. The cost of computing the rotation through an angle β about the y-axis, however, requires $O(p^3)$ work even if the coefficients $\{d_n^{m',m}(\beta)\}$ were given.

2. Recurrence relations

Assuming the rotations matrices have not been precomputed and stored, it is the calculation of the entries $\{d_n^{m',m}(\beta)\}$ themselves that dominates the cost of spherical harmonic rotation. The Wigner formula (8) clearly requires $O(p^4)$ work (p operations for each of the p^3 matrix entries), and is also subject to numerical instability when implemented naively. As a result, existing methods have tended to rely on the use of recurrences to compute the matrix entries [1,2,5,6,9,11,14,16,17].

One such scheme is based on the three basic recurrence relations below. These can be derived using formula (3.83) from [1].

$$\begin{aligned} d_n^{m',m}(\beta) = {} & \cos^2\left(\frac{\beta}{2}\right)\sqrt{\frac{(n+m)(n+m-1)}{(n+m')(n+m'-1)}}\, d_{n-1}^{m'-1,m-1}(\beta) - 2\sin\left(\frac{\beta}{2}\right)\cos\left(\frac{\beta}{2}\right)\sqrt{\frac{(n+m)(n-m)}{(n+m')(n+m'-1)}}\, d_{n-1}^{m'-1,m}(\beta) \\ & + \sin^2\left(\frac{\beta}{2}\right)\sqrt{\frac{(n-m)(n-m-1)}{(n+m')(n+m'-1)}}\, d_{n-1}^{m'-1,m+1}(\beta), \end{aligned} \tag{9}$$

$$d_n^{m',m}(\beta) = \sin^2\left(\frac{\beta}{2}\right)\sqrt{\frac{(n+m)(n+m-1)}{(n-m')(n-m'-1)}}d_{n-1}^{m'+1,m-1}(\beta) + 2\sin\left(\frac{\beta}{2}\right)\cos\left(\frac{\beta}{2}\right)\sqrt{\frac{(n+m)(n-m)}{(n-m')(n-m'-1)}}d_{n-1}^{m'+1,m}(\beta) + \cos^2\left(\frac{\beta}{2}\right)\sqrt{\frac{(n-m)(n-m-1)}{(n-m')(n-m'-1)}}d_{n-1}^{m'+1,m+1}(\beta), \tag{10}$$

$$d_n^{m',m}(\beta) = \sin\left(\frac{\beta}{2}\right)\cos\left(\frac{\beta}{2}\right)\sqrt{\frac{(n+m)(n+m-1)}{(n+m')(n-m')}}d_{n-1}^{m',m-1}(\beta) + \left(\cos^2\left(\frac{\beta}{2}\right) - \sin^2\left(\frac{\beta}{2}\right)\right)\sqrt{\frac{(n-m)(n+m)}{(n-m')(n+m')}}d_{n-1}^{m',m}(\beta) - \sin\left(\frac{\beta}{2}\right)\cos\left(\frac{\beta}{2}\right)\sqrt{\frac{(n-m)(n-m+1)}{(n-m')(n+m')}}d_{n-1}^{m',m+1}(\beta). \tag{11}$$

It is straightforward to compute $d_n^{m',m}(\beta)$ from (9)–(11), and we have used these recurrences in our FMM implementations [4,8] for more than a decade. They require only $O(p^3)$ work and, for expansions up to degree 40, encounter no significant numerical difficulties. We recently became interested, however, in some multiple scattering calculations [10] which involve spheres one or two hundred wavelengths in size, requiring expansions of degree up to one thousand or so. All of the recurrence-based schemes of which we are aware begin to lose significant accuracy once p reaches about one hundred and have no digits of accuracy once p equals two hundred.

Remark 2.1. It is worth noting that the full rotation operator can be applied using only $O(p^2)$ storage, although the work scales as $O(p^3)$. This follows from the fact that (9)–(11) describe a two-term recurrence in the degree n. Thus, two matrices of size $p \times p$ provide sufficient temporary storage, so long as one is willing to carry out the recurrence each time the operator is to be applied.

Before turning to our pseudospectral projection-based scheme, it is useful to define a suitable measure of accuracy. We have chosen to compute the L_2 norm of the error in rotating the multipole moments of degree n:

$$E = \frac{\sum_{m=-n}^{n}|M_n^{m'} - \mathcal{M}_n^{m'}|^2}{\sum_{m=-n}^{n}|\mathcal{M}_n^{m'}|^2}, \tag{12}$$

where $\mathcal{M}_n^{m'}$ denotes the exact value of the rotated expansion coefficient. For data, we first compute the outgoing multipole coefficients due to a Helmholtz (acoustic) source at $\left(1/\sqrt{2}, 1/\sqrt{2}, 0\right)$ with unit strength:

$$M_n^m = j_n(k)Y_n^m(\pi/2, \pi/4),$$

with the Helmholtz parameter $k = p$, where $j_n(k)$ denotes the spherical Bessel function of degree n and p is the degree of the truncated expansion. By rotating the source location, it is straightforward to compute the exact coefficients $\mathcal{M}_n^{m'}$.

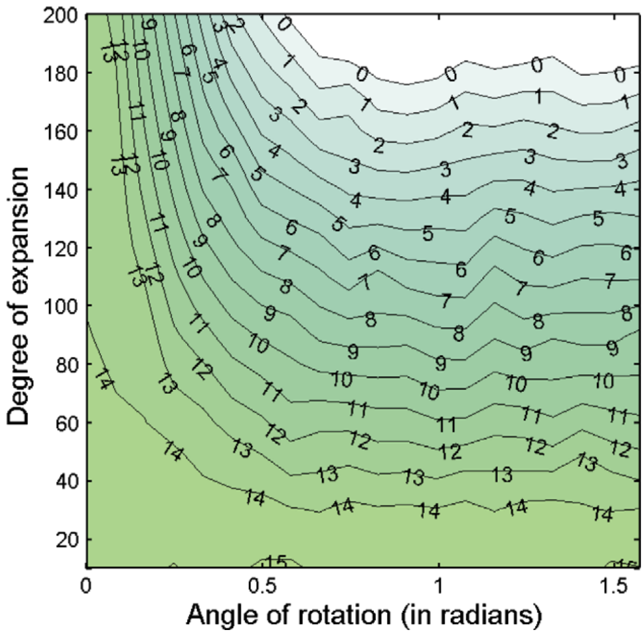

Fig. 1. A plot of accuracy as a function of expansion degree (y-axis) and rotation angle (x-axis). Shown are the contours of $-\log_{10}(E)$ with E defined in (12) - that is, the number of digits of accuracy.

The performance of the recurrence is plotted in Fig. 1 using 64-bit arithmetic. The x-axis denotes the angle of rotation and the y-axis denotes the degree of the expansion. The contours show the number of digits of accuracy in using the recurrences (9)–(11). Note that for expansions of degree 40, the results are accurate to 13 digits, that at degree 100 the results are accurate to about 8 digits, and that at degree 180 all accuracy is lost.

Remark 2.2. It should be noted that errors in rotation don't translate directly into errors in evaluating the field from a rotated expansion. In a resolved multipole expansion, the high order modes have decayed rapidly and mask the error for a time. Once the 100th mode is making a significant contribution however, the 8 digit loss will be manifested, and once the 180th mode is making a significant contribution, the loss of accuracy will be seen in the field evaluation as well.

Similar results (or worse) are obtained for all the recurrence schemes we tested.

3. Rotation via pseudospectral projection

In order to derive a stable scheme, consider the unit sphere rotated by an angle β about the y-axis (Fig. 2). An elementary calculation shows that in the new coordinate system

$$(x,y,z) \to (x',y',z') = (\cos\beta x - \sin\beta z, y, \sin\beta x + \cos\beta z).$$

The inverse mapping is given by

$$(x',y',z') \to (x,y,z) = (\cos\beta x' + \sin\beta z', y', -\sin\beta x' + \cos\beta z').$$

We denote the rotated equator by Γ, parameterized in the rotated frame as

$$\Gamma = (\cos\phi', \sin\phi', 0), \quad \phi' \in [0, 2\pi].$$

Definition 3.1. Let $\underline{\theta}'$ denote the unit vector in the θ' direction on the equator of the rotated sphere (Fig. 2):

$$\underline{\theta}' = (0,0,-1).$$

On Γ, we define the functions F_n and G_n by

$$F_n(\phi') \equiv F_n(\cos\phi', \sin\phi', 0) = \sum_{m=-n}^{n} M_n^m Y_n^m(\theta, \phi), \tag{13}$$

$$G_n(\phi') \equiv G_n(\cos\phi', \sin\phi', 0) = \frac{\partial F_n}{\partial \theta'}(\phi') = \nabla F_n(\phi') \cdot \underline{\theta}'. \tag{14}$$

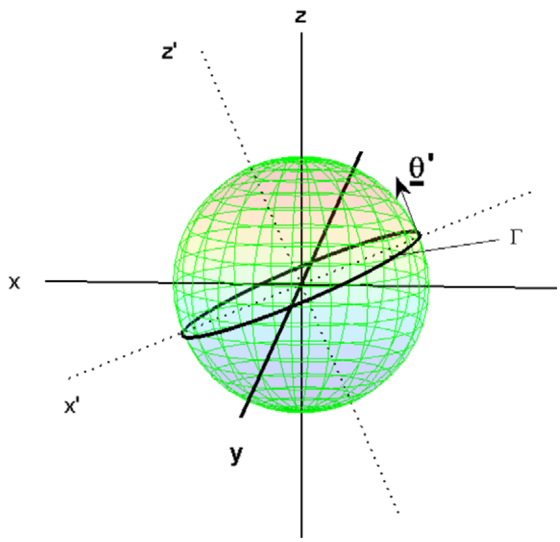

Fig. 2. A sphere rotated about the y-axis by an angle β. The x-axis is mapped to the x'-axis and the z-axis is mapped to z'-axis. Γ is the equator on the rotated sphere and $\underline{\theta}'$ is the unit vector in the θ' direction in the rotated frame.

Here, (θ,ϕ) denote the spherical coordinates in the original frame of the target point $P \in \Gamma$. Since $P = P_F = (\cos\phi', \sin\phi', 0)$ in the rotated frame, we can compute $P_E = (\cos\beta\cos\phi', \sin\phi', -\sin\beta\cos\phi')$ in the original frame, from which it is straightforward to compute (θ,ϕ).

Lemma 1. *Let F_n and G_n be given by (13) and let*

$$f_n^{m'} = \frac{1}{2\pi}\int_0^{2\pi} F_n(\phi')e^{-im'\phi'}d\phi', \qquad g_n^{m'} = \frac{1}{2\pi}\int_0^{2\pi} G_n(\phi')e^{-im'\phi'}d\phi'. \tag{15}$$

Then

$$M_n^{m'} = \frac{f_n^{m'}\widehat{P_n^{m'}}(0) + g_n^{m'}\widehat{Q_n^{m'}}(0)}{\widehat{P_n^{m'}}(0)^2 + \widehat{Q_n^{m'}}(0)^2}, \tag{16}$$

where

$$\widehat{P_n^m}(\cos\theta') = \sqrt{\frac{2n+1}{4\pi}}\sqrt{\frac{(n-|m|)!}{(n+|m|)!}}\cdot P_n^{|m|}(\cos\theta'),$$
$$\widehat{Q_n^m}(\cos\theta') = \sqrt{\frac{2n+1}{4\pi}}\sqrt{\frac{(n-|m|)!}{(n+|m|)!}}\cdot \frac{d}{d\theta'}P_n^{|m|}(\cos\theta').$$

Proof. We expand $F_n(\phi')$ as a spherical harmonic expansion in the rotated frame, with $\theta' = \pi/2$ on Γ so that $\cos\theta' = 0$:

$$F_n(\phi') = \sum_{m=-n}^{n} M_n^{m'}\widehat{P_n^{m'}}(0)e^{im'\phi}, \tag{17}$$

$$G_n(\phi') = \sum_{m=-n}^{n} M_n^{m'}\widehat{Q_n^{m'}}(0)e^{im'\phi}. \tag{18}$$

Fourier analysis of (17) and (18) yields

$$f_n^{m'} = M_n^{m'}\widehat{P_n^{m'}}(0),$$
$$g_n^{m'} = M_n^{m'}\widehat{Q_n^{m'}}(0),$$

and the result follows from solving these two equations for $M_n^{m'}$ in a least squares sense. □

Remark 3.1. The reason we use a least squares procedure is that for some values of n and m', one of $P_n^{m'}(0), Q_n^{m'}(0)$ vanishes. They never vanish simultaneously, so that the formula in Eq. (16) is always applicable.

Remark 3.2. By analogy with the literature on spectral methods, we refer to this scheme as *pseudospectral projection*. That is, in order to carry out a transformation in the spectral domain (spherical harmonic coefficients), we have mapped back to "physical space" (values on the rotated unit sphere) in an intermediate stage.

Remark 3.3. The integrands in (15) are band-limited so that the trapezoidal rule is exact so long as the number of quadrature nodes is greater than $2p$ [3].

Algorithm. Rotation via Pseudospectral Projection

1. Choose $2p+2$ equispaced nodes on Γ.
2. Compute the coordinates (θ,ϕ) of each node in the original coordinate system.
3. For each node, compute $F_n(\phi')$ and $G_n(\phi')$. (This requires the calculation of $Y_n^m(\theta,\phi)$ and its gradient at a cost of p^2 work per node.)
4. For $n = 0,\ldots,p$, use the FFT to compute $f_n^{m'}$ and $g_n^{m'}$.
5. Compute $M_n^{m'}$ using (16).

The total cost of the procedure is clearly $O(p^3)$. Stability is a consequence of the fact that we are simply using orthogonal projection of the function evaluated at equispaced points on the rotated equator. The experiment carried out in Section 2 using recurrence relations was repeated using the projection procedure described above, using 64-bit arithmetic. We plot the maximum of the error over all rotation angles as a function of expansion degree in Fig. 3. The number of digits of accuracy lost scales roughly with the logarithm of the expansion degree. At $p = 1000$, about 13 digits of accuracy were obtained for all rotation angles.

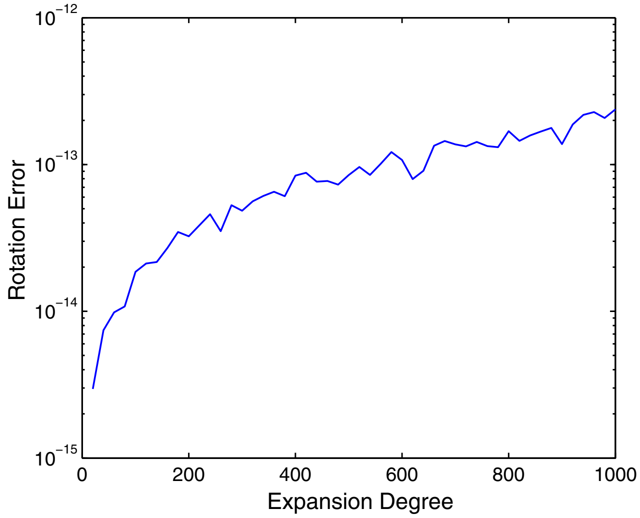

Fig. 3. A plot of error in rotation as a function of expansion degree using the projection-based scheme.

4. Conclusions

We have presented a simple scheme for rotating a spherical harmonic expansion of arbitrary degree p based on pseudo-spectral projection rather than the explicit construction of the rotation matrix. For low order expansions (up to $p = 40$ or so), either approach is satisfactory. The recurrence-based approach is, in our implementation, about twice as fast. On the other hand, in applications where p is significantly greater, the existing recurrence-based schemes break down while the projection-based scheme does not. Both approaches can be carried out using $O(p^2)$ storage. If the same rotation matrix is to be applied repeatedly and storage is not an issue, saving the values of $\widehat{P_n^{m'}}$ and $\widehat{Q_n^{m'}}$ at the quadrature nodes on the rotated equator Γ can save a factor of 3 in CPU time.

Because of the simplicity of the implementation, we expect the method to be of use in a variety of applications, especially high frequency scattering calculations.

Acknowledgments

The method described here grew out of several conversations with V. Rokhlin, whom we would like to thank.

Appendix A. Computation of $G_n(\phi')$

The computation of $G_n(\phi')$ in (14) is straightforward. In the original coordinate system,

$$\underline{\theta}' = (-\sin\beta, 0, -\cos\beta)$$

and

$$\nabla F_n = \left(\frac{\partial F_n}{\partial\theta}\frac{\partial\theta}{\partial x} + \frac{\partial F_n}{\partial\phi}\frac{\partial\phi}{\partial x}, \ \frac{\partial F_n}{\partial\theta}\frac{\partial\theta}{\partial y} + \frac{\partial F_n}{\partial\phi}\frac{\partial\phi}{\partial y}, \ \frac{\partial F_n}{\partial\theta}\frac{\partial\theta}{\partial z} + \frac{\partial F_n}{\partial\phi}\frac{\partial\phi}{\partial z}\right),$$

where

$$\frac{\partial\theta}{\partial x} = \cos\theta\cos\phi, \quad \frac{\partial\theta}{\partial y} = \cos\theta\sin\phi, \quad \frac{\partial\theta}{\partial z} = -\sin\theta,$$
$$\frac{\partial\phi}{\partial x} = -\sin\phi, \quad \frac{\partial\phi}{\partial y} = \cos\phi, \quad \frac{\partial\phi}{\partial z} = 0.$$

The quantities $\frac{\partial F_n}{\partial\theta}$ and $\frac{\partial F_n}{\partial\phi}$ are easily computed from the spherical harmonic representation (13).

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