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Note

Fast and Accurate Spectral Treatment of Coordinate Singularities

1. Introduction

In spherical and cylindrical geometries the coordinate singularities along the polar axis can decrease the accuracy or computational efficiency of classical spectral methods. This is due to the fact that analytic functions have special behavior near the singularities. Standard spectral representations either do not fully capture that behavior, or they are ill-suited for fast transforms and are therefore inefficient for computing products [1]. In this note we present algorithms that use modified spectral representations which explicitly enforce analyticity on the axis and use fast Fourier transforms to compute products.

2. Behavior Near the Singularity

Cylindrical and spherical coordinates both have singularities along their polar axes; however, a good numerical method should preserve the smoothness of a $\mathscr{C}^{\infty}$ physical solution despite the singularities. Consider the Fourier expansion of a scalar function in spherical coordinates

$$F(r, \theta, \phi) = \sum_{m=-\infty}^{+\infty} \sum_{n=0}^{+\infty} F_{nm}(r) \cos(n\theta)\, e^{im\phi} \tag{1}$$

and in cylindrical coordinates

$$F(s, z, \phi) = \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} F_{nm}(s)\, e^{inz} e^{im\phi}, \tag{2}$$

where we limit this discussion to a bounded domain in r and s and choose units such that $0 \leqslant r \leqslant 1$, $0 \leqslant \theta \leqslant \pi$, $0 \leqslant \phi \leqslant 2\pi$, $0 \leqslant s \leqslant 1$, and $-\infty \leqslant z \leqslant +\infty$. It can be shown [1] that for F to be infinitely differentiable the spectral coefficients must satisfy

$$\sum_{n=0}^{+\infty} F_{nm}(r) \cos(n\theta) = O(\sin^{|m|} \theta) \qquad (\theta \to 0, \pi) \tag{3}$$

$$F_{nm}(r) = O(r^{|n|}) \qquad (r \to 0) \tag{4}$$

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and

$$F_{nm}(s) = O(s^{|m|}) \qquad (s \to 0). \tag{5}$$

Equations (3), (4), and (5) are the pole conditions and express the necessary and sufficient conditions for a solution to be $\mathscr{C}^\infty$. If these constraints are not satisfied, then the numerical method can create non-smooth solutions. All of the pole conditions are similar, and the treatment of one can easily be generalized to the others. (See Appendix.) Therefore, we shall treat only the $m = 0$ pole condition in Eq. (4)—the singularity in axisymmetric spherical coordinates. An expansion that automatically enforces this pole condition is

$$F(r, \theta) = \sum_{n=0}^{+\infty} F_n(r)\, r^n \cos(n\theta), \tag{6}$$

where $F_n(r)$ remains bounded at $r \to 0$. The basis functions used in this expansion are referred to as the modified Robert functions [2, 3], and we will refer to $F_n(r)$ as the nth Robert coefficient. Unfortunately, solving for $F_n(r)$ from $F(r, \theta)$ by dividing the inverse Fourier transform of $F(r, \theta)$ by r^n is ill-conditioned at $r \to 0$ [2]. Orszag, in an initial-value study, used an expansion that satisfies Eq. (4) for the first few n modes, and although the method allows the use of fast transforms, the maximum time-step is restricted [1]. Another approach to the pole problem, frequently used for (but not limited to) non-axisymmetric functions defined on spherical shells is to expand the θ–ϕ-dependence in spherical harmonics. Then pole condition (3) is automatically satisfied. This technique however, is not amenable to fast transforms and is consequently slower than the double Fourier series expansion [1]. Here, we present an algorithm that allows fast transforms with modified Robert functions.

3. Algorithm

Consider two axisymmetric functions $U(r, \theta)$ and $V(r, \theta)$. Our goal is to compute $W \equiv UV$ in a well-conditioned manner that exploits fast transforms in the θ direction. All three quantities can be written in the Robert form:

$$U(r, \theta) = \sum_{m=0}^{+\infty} U_m(r)\, r^m \cos(m\theta) \tag{7}$$

$$V(r, \theta) = \sum_{m=0}^{+\infty} V_m(r)\, r^m \cos(m\theta) \tag{8}$$

$$W(r, \theta) = \sum_{m=0}^{+\infty} W_m(r)\, r^m \cos(m\theta). \tag{9}$$

In what follows, it is assumed that we know how to compute products of $U_{m_1}(r)$ and $V_{m_2}(r)$ in a well-conditioned, fast manner due to the fact that U_{m_1} and V_{m_2} are regular, smooth functions of r that need not satisfy any pole conditions (i.e., for the purposes of this paper, we can assume that $U_{m_1}(r)$ and $V_{m_2}(r)$ are known at grid or collocation points and their products are computed by direct multiplication). When computing such products, we ignore the effects of truncation errors.

We define the auxiliary functions:

$$U1^{(c)}(r,\theta) \equiv \sum_{m=0}^{+\infty} U_m(r)\cos(m\theta) \tag{10}$$

$$V1^{(c)}(r,\theta) \equiv \sum_{m=0}^{+\infty} V_m(r)\cos(m\theta) \tag{11}$$

$$U1^{(s)}(r,\theta) \equiv \sum_{m=0}^{+\infty} U_m(r)\sin(m\theta) \tag{12}$$

$$V1^{(s)}(r,\theta) \equiv \sum_{m=0}^{+\infty} V_m(r)\sin(m\theta) \tag{13}$$

$$U2^{(c)}(r,\theta) \equiv \sum_{m=0}^{+\infty} U_m(r)\, r^{2m}\cos(m\theta) \tag{14}$$

$$V2^{(c)}(r,\theta) \equiv \sum_{m=0}^{+\infty} V_m(r)\, r^{2m}\cos(m\theta) \tag{15}$$

$$U2^{(s)}(r,\theta) \equiv \sum_{m=0}^{+\infty} U_m(r)\, r^{2m}\sin(m\theta) \tag{16}$$

$$V2^{(s)}(r,\theta) \equiv \sum_{m=0}^{+\infty} V_m(r)\, r^{2m}\sin(m\theta). \tag{17}$$

Now write W as the double sum:

$$W = \sum_{m_1=0}^{+\infty}\sum_{m_2=0}^{+\infty} U_{m_1} V_{m_2} r^{m_1+m_2}\cos(m_1\theta)\cos(m_2\theta) \tag{18}$$

or

$$W = \frac{W1 + W2}{2}, \tag{19}$$

where

$$W1 \equiv \sum_{m_1=0}^{+\infty}\sum_{m_2=0}^{+\infty} U_{m_1} V_{m_2} r^{m_1+m_2}\cos(m_1+m_2)\theta \tag{20}$$

$$W2 \equiv \sum_{m_1=0}^{+\infty}\sum_{m_2=0}^{+\infty} U_{m_1} V_{m_2} r^{m_1+m_2}\cos(m_1-m_2)\theta. \tag{21}$$

We now show that the Robert coefficients of $W1$ and $W2$ can be derived from the Fourier coefficients of suitably chosen products of our auxiliary functions, which can themselves be computed by fast Fourier transforms (FFTs). We start with $W1$:

$$W1(r, \theta) = \sum_{m=0}^{+\infty} \left(\sum_{m_1=0}^{m} U_{m_1} V_{m-m_1} \right) r^m \cos(m\theta) = \sum_{m=0}^{+\infty} W1_m(r)\, r^m \cos(m\theta) \quad (22)$$

However,

$$U1^{(c)}V1^{(c)} - U1^{(s)}V1^{(s)} = \sum_{m_1, m_2=0}^{+\infty} U_{m_1} V_{m_2} \cos(m_1 + m_2)\theta \quad (23)$$

so that

$$U1^{(c)}V1^{(c)} - U1^{(s)}V1^{(s)} = \sum_{m=0}^{+\infty} W1_m \cos(m\theta). \quad (24)$$

Therefore the Robert coefficient $W1_m$ is the inverse Fourier transform of $U1^{(c)}V1^{(c)} - U1^{(s)}V1^{(s)}$.

To obtain $W2_m$, the procedure is a bit more complicated but is based on the same principle. We write

$$W2 = \sum_{m=0}^{+\infty} W2_m r^m \cos(m\theta). \quad (25)$$

Equations (21) and (25) show that

$$W2_m = c_m \sum_{m_1=0}^{+\infty} (U_{m+m_1} V_{m_1} + V_{m+m_1} U_{m_1})\, r^{2m_1} \quad (26)$$

and

$$c_m = \begin{cases} 1 & \text{if } m > 0 \\ 1/2 & \text{if } m = 0. \end{cases} \quad (27)$$

But again, we can make use of our auxiliary functions,

$$U1^{(c)}V2^{(c)} + U1^{(s)}V2^{(s)} + V1^{(c)}U2^{(c)} + V1^{(s)}U2^{(s)}$$
$$= \sum_{m=0}^{+\infty} W2_m(r)(1 + r^{2m}) \cos(m\theta). \quad (28)$$

To obtain $W2_m$, we then divide the inverse Fourier transform of the left-hand side of Eq. (28) by $(1 + r^{2m})$ which is well-conditioned because $1 \leqslant (1 + r^{2m}) \leqslant 2$. In this algorithm, eight FFTs are needed to obtain the values of the auxiliary functions at the collocation points, and two inverse transforms are needed to retrieve $W1_m$ and

$W2_m$. A modification of our method requires only one inverse transform if we note that

$$U1^{(c)}V1^{(c)} - U1^{(s)}V1^{(s)} + U2^{(c)}V2^{(c)} - U2^{(s)}V2^{(s)}$$
$$= \sum_{m=0}^{+\infty} W1_m(r)(1+r^{2m})\cos(m\theta). \tag{29}$$

Then Eqs. (28) and (29) imply

$$U1^{(c)}V2^{(c)} + U1^{(s)}V2^{(s)} + V1^{(c)}U2^{(c)} + V1^{(s)}U2^{(s)} + U1^{(c)}V1^{(c)}$$
$$- U1^{(s)}V1^{(s)} + U2^{(c)}V2^{(c)} - U2^{(s)}V2^{(s)}$$
$$= 2\sum_{m=0}^{+\infty} W_m(r)(1+r^{2m})\cos(m\theta). \tag{30}$$

Here, the Robert coefficients $W_m(r)$ are obtained directly by dividing the inverse transform of Eq. (30) by $(1+r^{2m})$.

4. Conclusion

Our fast convolution algorithm uses modified Robert functions is well-conditioned and requires nine FFTs in the θ direction. In contrast, spherical harmonics do not have efficient fast transforms. Orszag's double Fourier series method requires only three FFTs but does not satisfy all of the pole conditions. We have implemented our algorithm in an axisymmetric spherical geometry for a set of hydrodynamic equations with fourth-order spatial derivatives (which causes stiffness at the origin). Our fast convolution method is stable and gives accurate solutions, whereas we found that the Fourier series method failed. This application of our method will be reported elsewhere.

Our derivation is easily extentable to other geomtries, and in the Appendix we present it for pole conditions (3) and (4). In three-dimensional non-axisymmetric spherical geometries, there is a double coordinate singularity at $r=0$ and $\theta = 0, \pi$. Treating it requires 16 auxiliary functions and 17 FFTs, hence the method is six times slower than the Fourier series method (and might be as slow as the spherical harmonics expansion when only a small number of θ modes are used). Another limitation of our method is that nonlinear terms other than products cannot be computed. Higher-order products can be calculated by repeated application of the algorithm, but the method is costly.

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APPENDIX A

Here, we give the derivation of the convolution algorithm in the case where the representation is of the form

$$F(\theta, \phi) = \sum_{m=-\infty}^{+\infty} F_m(\theta) \sin^{|m|} \theta e^{im\phi} \tag{31}$$

which is the expansion that automatically satisfies the pole condition (3) on a spherical shell. It is also the appropriate expansion in cylindrical geometry by substituting s for $\sin \theta$. Again, our goal is to compute the Robert coefficients of $W \equiv UV$. We write

$$U(\theta, \phi) = \sum_{m=-\infty}^{+\infty} U_m(\theta) \sin^{|m|} \theta e^{im\phi} \tag{32}$$

$$V(\theta, \phi) = \sum_{m=-\infty}^{+\infty} V_m(\theta) \sin^{|m|} \theta e^{im\phi} \tag{33}$$

$$W(\theta, \phi) = \sum_{m=-\infty}^{+\infty} W_m(\theta) \sin^{|m|} \theta e^{im\phi} \tag{34}$$

and define the functions

$$\overline{U1}(\theta, \phi) \equiv \sum_{m=0}^{+\infty} c_m U_m(\theta)\, e^{im\phi} \tag{35}$$

$$\overline{U2}(\theta, \phi) \equiv \sum_{m=0}^{+\infty} c_m U_m(\theta) \sin^{|2m|} \theta e^{im\phi} \tag{36}$$

$$\widehat{U1}(\theta, \phi) \equiv \sum_{m-\infty}^{0} c_m U_m(\theta)\, e^{im\phi} \tag{37}$$

$$\widehat{U2}(\theta, \phi) \equiv \sum_{m=-\infty}^{0} c_m U_m(\theta) \sin^{|2m|} \theta e^{im\phi} \tag{38}$$

$$\overline{V1}(\theta, \phi) \equiv \sum_{m=0}^{+\infty} c_m V_m(\theta)\, e^{im\phi} \tag{39}$$

$$\overline{V2}(\theta, \phi) \equiv \sum_{m=0}^{+\infty} c_m V_m(\theta) \sin^{|2m|} \theta e^{im\phi} \tag{40}$$

$$\widehat{V1}(\theta, \phi) \equiv \sum_{m-\infty}^{0} c_m V_m(\theta)\, e^{im\phi} \tag{41}$$

$$\widehat{V2}(\theta, \phi) \equiv \sum_{m=-\infty}^{0} c_m V_m(\theta) \sin^{|2m|} \theta e^{im\phi}. \tag{42}$$

The product UV can be decomposed into four terms:

$$W = W1 + W2 + W3 + W4, \tag{43}$$

where

$$W1 \equiv \sum_{m_1=0}^{+\infty} \sum_{m_2=0}^{+\infty} c_{m_1} U_{m_1} c_{m_2} V_{m_2} \sin^{|m_1|+|m_2|} \theta e^{i(m_1+m_2)\phi} \tag{44}$$

$$W2 \equiv \sum_{m_1=-\infty}^{0} \sum_{m_2=-\infty}^{0} c_{m_1} U_{m_1} c_{m_2} V_{m_2} \sin^{|m_1|+|m_2|} \theta e^{i(m_1+m_2)\phi} \tag{45}$$

$$W3 \equiv \sum_{m_1=-\infty}^{0} \sum_{m_2=0}^{+\infty} c_{m_1} U_{m_1} c_{m_2} V_{m_2} \sin^{|m_1|+|m_2|} \theta e^{i(m_1+m_2)\phi} \tag{46}$$

$$W4 \equiv \sum_{m_1=0}^{+\infty} \sum_{m_2=-\infty}^{0} c_{m_1} U_{m_1} c_{m_2} V_{m_2} \sin^{|m_1|+|m_2|} \theta e^{i(m_1+m_2)\phi}. \tag{47}$$

Let $W1_m$, $W2_m$, $W3_m$, $W4_m$ be the Robert coefficients of $W1$, $W2$, $W3$, $W4$, respectively. We can easily obtain $W1_m + W2_m$ from the identity

$$\overline{U1}\,\overline{V1} + \widehat{U1}\widehat{V1} = \sum_{m=-\infty}^{+\infty} (W1_m + W2_m)\, e^{im\phi}. \tag{48}$$

Similar to the derivation in Section 3, we do not compute $(W3_m + W4_m)$ directly but rather $(W3_m + W4_m)(1 + \sin^{|2m|} \theta)$:

$$\overline{U1}\widehat{V2} + \widehat{U1}\overline{V2} + \overline{V1}\widehat{U2} + \widehat{V1}\overline{U2} = \sum_{m=-\infty}^{+\infty} (W3_m + W4_m)(1 + \sin^{|2m|} \theta)\, e^{im\phi}. \tag{49}$$

Again, we can reduce the number of inverse transforms from 2 to 1 by computing $(1 + \sin^{|2m|} \theta)\, W_m$ instead of $(W1_m + W2_m)$ and $(1 + \sin^{|2m|} \theta)(W3_m + W4_m)$. This is achieved by noticing that

$$\overline{U1}\,\overline{V1} + \widehat{U1}\widehat{V1} + \overline{U2}\,\overline{V2} + \widehat{U2}\widehat{V2} = \sum_{m=-\infty}^{+\infty} (W1_m + W2_m)(1 + \sin^{|2m|} \theta)\, e^{im\phi}. \tag{50}$$

This method now requires eight direct FFTs and one inverse FFT.

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