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Spectral radial basis functions for full sphere computations

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Abstract

The singularity of cylindrical or spherical coordinate systems at the origin imposes certain regularity conditions on the spectral expansion of any infinitely differentiable function. There are two efficient choices of a set of radial basis functions suitable for discretising the solution of a partial differential equation posed in either such geometry. One choice is methods based on standard Chebyshev polynomials; although these may be efficiently computed using fast transforms, differentiability to all orders of the obtained solution at the origin is not guaranteed. The second is the so-called one-sided Jacobi polynomials that explicitly satisfy the required behavioural conditions. In this paper, we compare these two approaches in their accuracy, differentiability and computational speed. We find that the most accurate and concise representation is in terms of one-sided Jacobi polynomials. However, due to the lack of a competitive fast transform, Chebyshev methods may be a better choice for some computationally intensive timestepping problems and indeed will yield sufficiently (although not infinitely) differentiable solutions provided they are adequately converged.

Keywords: Coordinate singularity; Jacobi polynomials; Chebyshev polynomial; Spectral method; Polar coordinates

1. Introduction

In a cylindrical or spherical geometry, the origin is a singular point. This is manifested not only in the convergence of grid points in many numerical schemes severely restricting tractable timesteps, but in certain regularity conditions that any solution must satisfy in order to remain differentiable to all orders at the origin. This issue may be regarded in a positive or negative light depending on the point of view. On the one hand, one may be concerned that any numerically derived function might not be sufficiently differentiable (and therefore will not be physically meaningful) at the origin; on the other, the extra constraints may be exploited to hone the numerical scheme and consequently speed up convergence. A thorough review of these issues may be found in [1].

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In a 2D polar geometry, any smooth (i.e. infinitely differentiable) function $f(r,\phi)$, depending on the radius $r\in[0,1]$ and polar angle $\phi\in[0,2\pi]$ has a Fourier expansion of the form

$$f(r,\phi)=\sum_n \mathrm{e}^{\mathrm{i}n\phi}f_n(r),\quad f_n(r)=r^n g_n(r),$$

where the rightmost equation expresses the regularity condition and $g_n(r)$ is necessarily itself both even and smooth [1–3]. Similarly in the spherical case, an expansion in terms of spherical harmonics $Y_l^m(\cos\theta)\mathrm{e}^{\mathrm{i}m\phi}$ where (θ,ϕ) are respectively colatitude and longitude implies that the multiplying radial function must be of the form $r^l g_{lm}(r)$. Thus in both cases (and for the remainder of this paper) we may speak of the regularity condition being that $f_l(r)=r^l g_l(r)$ (with g_l smooth and even), although the physical interpretation of the wavenumber l (referring either to polar angle or colatitude) depends on the coordinate system. An immediate consequence of the regularity condition is that each radial function has a definite parity, a property that in fact may be derived independently of differentiability by, for example, identifying the point $(-r,\phi+\pi)$ with (r,ϕ) in plane polar coordinates [4]; an analogous result holds in the spherical polar case. Note that the parity and regularity conditions are neither required nor in general satisfied by any solution on a domain that excludes the origin.

Any smooth solution of a partial differential equation automatically satisfies the regularity conditions. It follows that any solution produced by a convergent numerical scheme will also satisfy these conditions, at least in the limit of infinite truncation and infinite precision. In practice however, highly differentiable solutions will only be obtained in general with numerical schemes that converge quickly in truncation level, for the imprecision caused by the accumulation of roundoff errors will violate the regularity conditions.

Methods based on Chebyshev expansions, both in spectral [5–8] and interpolation [9–12] forms have been widely used to represent the radial structure, the major advantage being the availability of a fast transform (FFT). The potential clustering of the associated grid points in physical space close to the origin may be removed by either expanding over the double interval $[-1,1]$ (rather than $[0,1]$ with the concomitant halving of the angular extent) or by exploiting their parity. However, in order to satisfy the regularity conditions at the origin, the Chebyshev polynomials must effect a perfect cancellation of all monomial terms of the form r^i with $i<l$. Assuming that the unknown solution has a nonzero projection onto each Chebyshev polynomial (which might be exponentially small) and noting that each Chebyshev polynomial $T_n(r)$ has a nonzero projection onto all monomials r^i of the same parity and degree $i<n$, regularity will never be achieved exactly at any given finite truncation. This therefore raises the question of how much the differentiability of the solution at the origin is compromised using such a method. One of the aims of this paper, addressed in Section 2, is to tackle this very question – to determine whether or not such a Chebyshev scheme provides a regular solution, or at least one that is sufficiently regular. Precisely how regular a solution needs to be to remain physically meaningful will depend on the problem: for most cases, only the first few derivatives need to be everywhere smooth; for others, the solution may need to be infinitely differentiable.

In such methods, regularity may be significantly affected by numerical imprecision introduced through the accumulation of roundoff errors. An important related issue therefore is the speed of convergence of the numerical scheme. Gottlieb and Orszag [5] claimed that the coordinate singularity degraded the convergence of Chebyshev methods and that introducing additional "pole" conditions (of the form $y'(0)=0$) speeded up convergence. In Section 2 we briefly revisit the issue of whether such extra conditions are required with our implementation.

An alternative method is to expand the unknown function in a radial basis that automatically satisfies all regularity conditions. The effect of roundoff error or otherwise lack of convergence can never degrade the differentiability which is guaranteed to all orders. In addition, the fact that the correct behaviour at the origin is built into the basis may significantly accelerate global convergence. One natural choice are Bessel (or spherical Bessel) functions being the radial part of the separable solution to the Helmholtz equation $\nabla^2 f+\lambda^2 f=0$. However, Bessel functions are not solutions of a sufficiently singular Sturm–Liouville problem [13,5] and therefore only achieve algebraic convergence (as attested by [14]). Nevertheless, Bessel functions have been used successfully in certain applications e.g. [15]. It is worth noting that the same algebraic convergence is also obtained when using Fourier series on a non-periodic domain [16]. A further option are the Poincaré polynomials, eigenfunctions of the inertial wave equation in 3D [17] although again there is no reason to suspect that