Spectral collocation methods for solution of Einstein's equations in null quasi-spherical coordinates*

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Abstract

The spectral methods which are being used to solve Einstein's equations in null quasi-spherical coordinates are described. They include Fast Fourier methods for evaluating derivatives in a uniform grid representation and methods for transforming to and from spin-weighted spherical harmonic representations. In theory, expressions involving spherical harmonics up to any fixed maximum angular momentum L can be routinely manipulated with accuracy depending only on the machine precision. The code we have running uses $L = 15$ or $L = 31$, with no assumed symmetries.

1. Introduction

The structure of Einstein's equations in null quasi-spherical (NQS) coordinates has been discussed in [1], these proceedings. Recall that NQS coordinates $\{z, r, \vartheta, \varphi\}$ satisfy the following conditions:

(1) The 3-surfaces $z =$ const. are null.

(2) The 2-surfaces $z =$ const., $r =$ const. are metric 2-spheres of area $4\pi r$.

(3) $\{\vartheta, \varphi\}$ are standard polar coordinates on these 2-spheres.

Because NQS coordinates foliate space-time by metric 2-spheres, Einstein's equations are naturally expressed in terms of spin-weighted functions on S^2 and the covariant differential operator edth [2], given by

$$\eth\eta = \frac{1}{\sqrt{2}} \sin^s\vartheta (\frac{\partial}{\partial\vartheta} - \frac{i}{\sin\vartheta}\frac{\partial}{\partial\varphi})(\eta \sin^{-s}\vartheta)\,, \tag{1}$$

for η of spin weight s.

Spectral collocation using spin-weighted spherical harmonics as basis functions then presents itself as a natural choice of numerical method for solving Einstein's equations in NQS coordinates.

*This is joint work with Prof. Robert Bartnik.

This paper describes how expressions such as (1) can be evaluated using fast Fourier methods and how one can efficiently transform between representations of a spin-weighted function in terms of its spherical harmonic components and the values it takes on a regular grid of collocation points on S^2.

2. The NQS solution algorithm

The central role played by the spectral techniques to be described is best illustrated by briefly reviewing the algorithm being used to solve the characteristic initial value problem (CIVP) in NQS coordinates.

In the CIVP we are given a spin 1 field β as initial data on a null surface z = const. Numerical solution of Einstein's equations amounts to evolving β from one z = const. slice to the next. This involves 3 steps:

Step 1

On the null z = const. slice one solves for four auxiliary fields, H, Q^-, J and K. These fields (which are defined in [1]) are of spins 0,1,0 and 2 respectively, and will be denoted here collectively as y^i, $i = 1, \ldots, 6$ (Q^- and K have both real and imaginary parts). The system of PDEs to be solved is then of the form

$$\frac{\partial y^i}{\partial r} = f^i(r,\ \vartheta,\ \varphi,\ \partial y^i/\partial\vartheta,\ \partial y^i/\partial\varphi)\,, \tag{2}$$

where the f^i depend on r, ϑ, φ both explicitly and through the field β and its 1st and 2nd covariant angular derivatives (terms such as div β and $\eth$ curl β).

These PDEs are solved by spectral collocation [3] using an explicit integration scheme. For fixed radius r, the fields y^i are represented by the values they take on a collocation grid on S^2. The S^2 grid is equally spaced in the polar angles ϑ and φ, and is typically of size 16×32 or 32×64, with the poles ($\vartheta = 0, \pi$) being midway between grid points. Note that the spatial resolutions in the ϑ and φ directions are equal at the equator for a grid of shape $N/2 \times N$.

The derivatives $\partial y/\partial\vartheta$ and $\partial y/\partial\varphi$ are evaluated on the S^2 grid using Fast Fourier Transforms (FFTs). One simply multiplies the Fourier coefficients of y by the appropriate wavenumber and then transforms back to obtain the grid values of the derivatives of y. The only complication is that taking the FFTs in the ϑ direction involves some care, as described in Section 3.

Once the values of the derivatives of y have been found, the functions f^i can be evaluated at the S^2 grid points. Equations (2) can then be integrated as a large system of $3N^2$ ODEs. At present a 4th order Runge-Kutta (RK4) method is being used, starting with prescribed initial data for y^i on a 2-sphere of non-zero radius.

Using an appropriately scaled radial grid, equations (2) can be integrated out to $r = \infty$. Typically the radial grid has 128, 256 or 512 steps.

Step 2

On the null $z =$ const. slice one then solves for a spin 1 field γ. The equation for γ is

$$\eth\gamma + \mathrm{div}\,\gamma\frac{\eth\beta}{2-\mathrm{div}\,\beta} \;=\; -K + J\frac{\eth\beta}{2-\mathrm{div}\,\beta}\,. \tag{3}$$

The source terms on the RHS are given by the solutions obtained in Step 1.

For fixed radius and β not too large, (3) is an elliptic equation on S^2. So we solve for γ on the null slice by solving, at each grid radius, an elliptic equation for gamma restricted to S^2.

The operator on the LHS of (3) has a 6 dimensional kernel corresponding to the 6 spherical harmonic components of γ having $\ell = 1,\ m = 0, \pm 1$. Choosing to set these components of γ to zero partially fixes the gauge freedom in the NQS coordinate system and enables us to change the independent variable from γ to Γ using $\gamma = \eth^{-1}\Gamma$ (with $\eth^{-1}$ now well defined). Equation (3) then becomes,

$$\Gamma + \mathrm{div}\,(\eth^{-1}\Gamma)\frac{\eth\beta}{2-\mathrm{div}\,\beta} \;=\; -K + J\frac{\eth\beta}{2-\mathrm{div}\,\beta}\,. \tag{4}$$

The advantage of (4) over (3) is that the operator in (4) is close to the identity. The corresponding discretised problem is therefore well suited to iterative matrix methods.

We use the conjugate gradient (CG) method, which is an iterative method applicable to matrix problems of the form $Ax = b$ with A symmetric positive definite. Accordingly we actually solve an associated self-adjoint equation obtained by applying to (4) the operator adjoint to that in (4) with respect to the L^2 norm on S^2.

Implementation of the above scheme requires several transformations between representations of fields by their spin-weighted spherical harmonic coefficients and by their values on the S^2 grid. For example, the operator $\eth^{-1}$ is a trivial multiplicative operator on spectral coefficients, whereas the source terms are given in terms of grid values. Moreover, several products have to be calculated in the grid representation.

Using the CG method to solve for the spin 2 spherical harmonic coefficients of Γ turns out to be extremely efficient, typically requiring fewer than 10 iterations of the CG algorithm for an S^2 grid of size $N/2 \times N = 16 \times 32$. On this size grid we resolve all components of Γ up to angular momentum $\ell = N/2 - 1 = 15$, so in this case we are solving for $2((\ell+1)^2 - 4) = 504$ spectral coefficients.

The scheme's effectiveness is in part due to having a good initial guess for γ to use as the starting point of the CG iterations, namely the solution found for Γ on the 2-sphere at the previous radial position.

Step 3

The field β is evolved to the next $z =$ const. slice by numerical integration of an expression for $\partial\beta/\partial z$ which involves the fields y^i, γ and $\partial\gamma/\partial r$. The radial derivative of γ is calculated numerically using spline methods [4].

The results reported in the talk accompanying paper [1] were obtained using explicit RK4 integration of $\partial\beta/\partial z$. Other methods remain to be investigated and the relations between maximum stable step size Δz and the angular and radial resolutions are still to be determined.

Transformations between spherical harmonic and S^2 grid representations are necessary in Step 3 because of the potential for instabilities of the z integration to develop near the poles of the coordinate system. In the following sections we shall see that the number of degrees of freedom in the grid representation is at least twice that of the corresponding spherical harmonic representation (by corresponding we mean only involving basis functions which do not alias on the S^2 grid). It follows that a transformation from the grid representation to the spherical harmonic representation actually involves a projection. This projection may be viewed as an S^2-spectral filter.

If a field is evolved in the grid value representation without periodic filtering to remove numerical noise, then the numerical solution can eventually fall apart at the poles because it has too many degrees of freedom.

3. FFT evaluation of angular derivatives

The S^2 grid is uniform in ϑ and φ so that FFT methods can be used to evaluate the ϑ and φ derivatives of a spin s field. For integer s the real and imaginary parts of a spin s field on S^2 are (up to a factor) equal to the two independent frame components of a completely symmetric tensor on S^2 [2]. These components may be discontinuous at the poles, so are not obviously suited to Fourier expansion in the ϑ direction.

The standard orthonormal frame on S^2 is $(e_1,\, e_2) = (\partial/\partial\vartheta,\, \frac{1}{\sin\vartheta}\partial/\partial\varphi)$, with $\vartheta \in [0,\pi]$ and $\varphi \in [0, 2\pi)$. Let $T = T^{j_1\cdots j_s} e_{j_1} \otimes \cdots \otimes e_{j_s}$ be a smooth tensor field on S^2. As one crosses through either of the poles both of the basis vectors e_1 and e_2 reverse direction, so if the number of factors in $e_{j_1} \otimes \cdots \otimes e_{j_s}$ is odd then the component functions $T^{j_1\cdots j_s}$ must change sign across the poles.

To Fourier transform $T^{j_1\cdots j_s}$ in the ϑ direction we first extend the domain of definition of $T^{j_1\cdots j_s}$ to $\vartheta \in [-\pi,\, \pi]$ in such a way that the resulting functions are smooth and of period 2π in ϑ. Using the 2π periodicity in φ, we define

$$T^{j_1\cdots j_s}(-\vartheta, \varphi) \;=\; (-1)^s T^{j_1\cdots j_s}(\vartheta, \varphi + \pi), \quad \vartheta \in [0, \pi]. \tag{5}$$

Derivatives of $T^{j_1\cdots j_s}$ with respect to ϑ can then be calculated just as for φ derivatives, with the proviso that the direction of increasing ϑ be properly taken into account.

The procedure just described extends the functions $T^{j_1\cdots j_s}$ so as to be defined on the torus $S^1 \times S^1$. In Section 4 we shall see that this is a useful interpretation of equation (5). Alternatively, one can view the same equation as simply the transformation law for components with respect to two different S^2 coordinate charts, one based on circles of latitude and one based on circles of longitude.

There remains the question of how the calculated FFT derivatives relate to those one would calculate using a spin-weighted spherical harmonic expansion of T.

We use a real basis of spin 0 spherical harmonics so that the even and odd parity components of a spin s field are easily distinguished (for $s = 1$ the even/odd decomposition is just the Helmholtz decomposition of a vector field into div-free and curl-free parts). Accordingly, let

$$F_m(\varphi) = \begin{cases} 1 & m = 0 \\ \sqrt{2}\cos m\varphi & m > 0 \\ \sqrt{2}\sin |m|\varphi & m < 0 \end{cases} \tag{6}$$

then the spin 0 basis we use is

$${}_0Y_{\ell m} = \overline{P}_{\ell m}(\vartheta) F_m(\varphi)\,, \tag{7}$$

where $\ell = 0, \ldots, L$ and $m = -\ell, \ldots, \ell$. The functions $\overline{P}_{\ell m}(\vartheta) = \overline{P}_{\ell |m|}(\vartheta)$ are related to the associated Legendre functions $P_{\ell m}$, by

$$\overline{P}_{\ell m}(\vartheta) = (-1)^m \sqrt{2\ell+1} \frac{(\ell - m)!}{(\ell + m)!} P_{\ell m}(\cos\vartheta)\,. \tag{8}$$

The associated Legendre functions with argument $\cos\vartheta$ are,

$$P_{\ell m}(\cos\vartheta) = \frac{(-1)^m}{2^\ell \ell!} \sin^m \vartheta \left[\frac{d^{\ell+m}}{dx^{l+m}} (x^2 - 1)^\ell \right]_{x=\cos\vartheta}\,. \tag{9}$$

Basis functions for spin $s > 0$ fields of even and odd parity are then given by ${}_sY_{\ell m}$ and $i\,{}_sY_{\ell m}$ respectively (using real coefficients), where

$${}_sY_{\ell m} = \frac{-\sqrt{2}}{\sqrt{(\ell+s)(l-s-1)}}\, \eth\, {}_{s-1}Y_{\ell m}\,,$$

with $\ell = s, s+1, \ldots, L$ and $m = -\ell, \ldots, \ell$. The spin-weighted spherical harmonics $\{{}_sY_{\ell m}\}$ are orthonormal with respect to the Hilbert norm on S^2,

$$\frac{1}{4\pi} \int_{S^2} {}_sY_{\ell_1 m_1}\, {}_s\overline{Y}_{\ell_2 m_2} \sin\vartheta d\vartheta d\varphi = \delta_{\ell_1 \ell_2} \delta_{m_1 m_2}\,, \quad s = 0, 1, \ldots$$

From (6)–(9) it is evident that the spin 0 harmonics ${}_0Y_{\ell m}$, are trigonometric polynomials in ϑ and φ. Using expression (1) for $\eth$, one can show that the ${}_sY_{\ell m}$ are likewise trigonometric polynomials, and can therefore be expressed as Fourier sums.

The highest wave number Fourier modes which occur in the set of basis functions $\{{}_sY_{\ell m} : s \le \ell \le L\}$ are $\cos(L\vartheta)$, $\sin(L\vartheta)$, $\cos(L\varphi)$, and $\sin(L\varphi)$. Therefore, on an S^2 grid of size $N/2 \times N$ the Fourier derivatives of ${}_sY_{\ell m}$ are *algebraically exact* for $\ell \le L = N/2 - 1$. Moreover, it is clear that amongst uniform S^2 grids, a grid of shape $N/2 \times N$ is optimal in terms of the number of spherical harmonics which can be represented on the grid without aliasing.

Because the Fourier derivatives of ${}_sY_{\ell m}$ are algebraically exact, the accuracy of FFT methods for evaluating expressions such as (1) depends only on the machine precision.

For example, the Laplacian of ${}_0Y_{\ell m}$ can be computed numerically using FFT methods and then compared with the exact result. Using double precision on a DEC Alpha it is found that for $N = 32$ we have $\max(\Delta_0 Y_{\ell m}/\ell(\ell+1) + {}_0Y_{\ell m}) < 2 \times 10^{-12}$ for all $|m| \leq \ell$ and $\ell \leq 15$, where the maximum is taken over the S^2 grid points. For $N = 64$ we have $\max(\Delta_0 Y_{\ell m}/\ell(\ell+1) + {}_0Y_{\ell m}) < 4 \times 10^{-11}$ for all $|m| \leq \ell$ and $\ell \leq 31$.

4. Projecting from grid to spherical harmonic representations

Projections for fields of spin 0, 1 and 2 are required for the steps outlined in Section 2. Only that for the spin 0 case is described here, those for higher spins being completely analogous.

The number of basis functions in the set $\{{}_0Y_{\ell m} : 0 \leq \ell \leq L\}$ is $(L+1)^2$. However, to represent these functions on a regular S^2 grid we require a grid of size $(L+1) \times 2(L+1)$. The spin 0 functions of angular momentum of at most L therefore form a subspace of dimension $(L+1)^2$ in a Fourier space of dimension $4(L+1)^2$. We shall construct a projection onto this subspace which is orthogonal with respect to the natural inner product in the Fourier space,

$$\langle f_1, f_2 \rangle = \frac{1}{4\pi^2} \int_0^{2\pi} \int_0^{2\pi} f_1(\vartheta, \varphi) f_2(\vartheta, \varphi) d\vartheta d\varphi \tag{10}$$

$$= \frac{1}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} f_1(\vartheta_i, \varphi_j) f_2(\vartheta_i, \varphi_j), \tag{11}$$

where $\{(\vartheta_i, \varphi_j) : i, j = 1, \ldots, N\}$ are grid points and $N = 2(L+1)$.

To make use of (11) we use (5) to extend functions defined on S^2 to functions defined on the torus $T^2 = S^1 \times S^1$. In particular, given any set of values $\{f_{ij} \in \mathbf{R} : i = 1, \ldots, N/2,\ j = 1, \ldots, N\}$ on the S^2 grid, we use (5) to extend this to a set of grid values on T^2. There is then a unique interpolating trigonometric polynomial f such that $f(\vartheta_i, \varphi_j) = f_{ij}$. We project f to the spin 0 subspace as follows.

The basis vectors for the spin 0 subspace are the ${}_0Y_{\ell m}$. These vectors are not orthonormal with respect to (10). In fact, the metric induced on the spin 0 subspace by that of the Fourier space is given by

$$\begin{aligned} G_{\ell m\, \ell' m'} &= \langle {}_0Y_{\ell m}, {}_0Y_{\ell' m'} \rangle \\ &= \langle \overline{P}_{\ell m}(\vartheta), \overline{P}_{\ell' m'}(\vartheta) \rangle \langle F_m(\varphi), F_{m'}(\varphi) \rangle \\ &= \langle \overline{P}_{\ell m}(\vartheta), \overline{P}_{\ell' m}(\vartheta) \rangle \, \delta_{mm'} \,. \end{aligned} \tag{12}$$

Here, the index pair ℓm (and $\ell' m'$) is to be regarded as a combined index which takes $(L+1)^2$ values. Moreover, the summation convention will be employed for repeated indices which appear both raised and lowered in the one term.

For fixed m, the inner product (12) of the $\overline{P}$ functions forms a matrix which we denote as

$$A_{(m)\ell\ell'} = \langle \overline{P}_{\ell m}(\vartheta), \overline{P}_{\ell' m}(\vartheta) \rangle \,.$$

These matrices are defined only for $|m| \le \ell \le L$ and $|m| \le \ell' \le L$, so are square and of size $(L+1-|m|) \times (L+1-|m|)$. Let the inverse matrix be denoted $A^{\ell\ell'}_{(m)}$. Then (12) becomes

$$G_{\ell m\ \ell' m'} = A_{(m)\ell\ell'} \delta_{mm'}\,, \tag{13}$$

and the components of the inverse metric are given by

$$G^{\ell m\ \ell' m'} = A^{\ell\ell'}_{(m)} \delta^{mm'}, \qquad \text{(no sum on } m). \tag{14}$$

The dual basis vectors for the spin 0 subspace are

$${}_0Y^{\ell m} = G^{\ell m\ \ell' m'}\,{}_0Y_{\ell' m'}\,, \tag{15}$$

and satisfy

$$\langle {}_0Y_{\ell m},\, {}_0Y^{\ell' m'} \rangle = \delta^{\ell'}_{\ell} \delta^{m'}_{m}\,.$$

The orthogonal projection of f onto the spin 0 subspace is then obtained as

$$\mathrm{proj}(f) = \langle f,\, {}_0Y^{\ell m} \rangle {}_0Y_{\ell m}\,.$$

The numbers

$$f^{\ell m} = \langle f,\, {}_0Y^{\ell m} \rangle\,, \tag{16}$$

are the spin 0 spherical harmonic coefficients (of the projection) of f.

To calculate the inner product (16), first note that using (7), (14) and (15) the dual basis vectors can be written as

$${}_0Y^{\ell m} = \overline{P}^{\ell m}(\vartheta) F^m(\varphi)\,, \tag{17}$$

(in analogy with (7)) where we have set

$$\begin{aligned} \overline{P}^{\ell m}(\vartheta) &= A^{\ell\ell'}_{(m)} \overline{P}_{\ell' m}(\vartheta)\,, \\ F^m(\varphi) &= F_{m'}(\varphi)\delta^{m' m}\,. \end{aligned} \tag{18}$$

By Fourier analysis of f in the φ direction one can write $f = \hat{f}^k(\vartheta) F_k(\varphi)$. In particular, by φ-FFT of $\{f_{ij}\}$ one obtains the numbers $\hat{f}^k(\vartheta_i)$. The spin 0 coefficients of f can then be evaluated using (11) and (17) as

$$\begin{aligned} f^{\ell m} &= \langle \hat{f}^k(\vartheta) F_k(\varphi),\, \overline{P}^{\ell m}(\vartheta) F^m(\varphi) \rangle \\ &= \langle \hat{f}^k(\vartheta),\, \overline{P}^{\ell m}(\vartheta) \rangle\, \delta^m_k \\ &= \langle \hat{f}^m(\vartheta),\, \overline{P}^{\ell m}(\vartheta) \rangle \\ &= \frac{1}{N} \sum_{i=1}^{N} \hat{f}^m(\vartheta_i) \overline{P}^{\ell m}(\vartheta_i)\,. \end{aligned} \tag{19}$$

Fortran subroutines for transforming between grid values and spherical harmonic coefficients have been written for maximum angular momentum $L = 7, 15$ and 31. The grid values $\overline{P}^{\ell m}(\vartheta_i)$ which appear in the sum (19) were pre-computed in multiple precision and written to file using REDUCE. The functions $\overline{P}^{\ell m}(\vartheta)$, defined by (18), were constructed symbolically using exact inversion of the matrices $A_{(m)\,\ell\ell'}$. This symbolic approach was feasible because the metric $G_{\ell m\;\ell' m'}$ factorised as the tensor product (13), thus allowing exact inversion of G using matrices of size at most $(L+1)\times(L+1)$ rather than $(L+1)^2\times(L+1)^2$.

The analysis of spin 1 and spin 2 grid functions into spherical harmonic coefficients is in essence the same as for spin 0, complicated only by the fact that the induced metric on the subspace factorises as a tensor product only in a complex (mixed parity) basis. Separating the even and odd parity coefficients therefore requires some extra book keeping.

Projections for scalar and vector fields on S^2 (i.e. for spins 0 and 1) have been given by Swarztrauber in [6],[7],[8]. They differ from ours in that the metric used is not the natural Fourier metric (10). However, they have the advantage that simple formulae are available for the functions analogous to our $\overline{P}^{\ell m}(\vartheta)$.

The synthesis of a spin 0 grid function $f_{ij} = f(\vartheta_i, \varphi_j)$ from its spherical harmonic coefficients $f^{\ell m}$ follows from

$$\begin{aligned} f &= f^{\ell m}\,{}_0Y_{\ell m}(\vartheta,\varphi) \\ &= f^{\ell m}\overline{P}_{\ell m}(\vartheta)F_m(\varphi)\,. \end{aligned}$$

One first forms the quantities

$$\hat{f}^m(\vartheta_i) = \sum_{\ell=|m|}^{L} f^{\ell m}\overline{P}_{\ell m}(\vartheta_i)\,, \qquad \text{(no sum on } m). \tag{20}$$

and then uses inverse FFTs in the φ direction to obtain

$$f_{ij} = \hat{f}^m(\vartheta_i)F_m(\varphi_j)\,.$$

The grid values of the functions $\overline{P}_{\ell m}$ in (20) were pre-computed in REDUCE. Synthesis for fields of spin 1 and 2 is similar to that for a spin 0 field.

5. Conclusions

A spectral method has been described for solving the characteristic initial value problem for Einstein's equations in null quasi-spherical coordinates. The method involves the use of both Fourier and spherical harmonic expansions of fields with spin-weights 0,1 and 2. Techniques have been developed for transforming a spin-weighted field between grid and spherical harmonic representations. Fortran subroutines which implement these techniques have been written for spin-weights 0, 1 and 2.

The code for solving the CIVP is at the stage where preliminary results are now becoming available. On a DEC Alpha workstation the CPU time required to evolve a solution from one $z =$ const. slice to the next is about 2 minutes on a 16×32 S^2 grid $(L = 15)$ using 128 radial positions.

The code has yet to be tested on known NQS exact solutions. Other tests will involve monitoring those components of the Einstein equations which are not being used to evolve the solution.

Acknowledgment

This work is supported by the ARC Large Grant, "Spectral Method for Numerical Modelling of Gravitational Radiation" (A6933046).

References

[1] R. Bartnik, *Einstein equations in NQS coordinates*, these proceedings.

[2] R. Penrose and W. Rindler, *Spinors and Space-time, Vol. 1*, Cambridge University Press, 1984.

[3] C. Canuto, M. Y. Hussaini, A. Quarteroni and T. A. Zang, *Spectral Methods in Fluid Mechanics*, Springer Series in Computational Physics, New York, 1988.

[4] A. H. Norton, *Finite difference operators for PDEs, based on sampling kernels for spline quasi-interpolation*, UNSW preprint, 1992.

[5] S. Orszag, *Fourier series on spheres*, Monthly Weather Review, 1974, **102**, 56–75.

[6] P. N. Swarztrauber, *On the spectral approximation of discrete scalar and vector functions on the sphere*, SIAM J. Numer. Anal. 1979, **16**, 934–949.

[7] P. N. Swarztrauber, *The approximation of vector functions and their derivatives on the sphere*, SIAM J. Numer. Anal. 1979, **16**, 934–949.

[8] P. N. Swarztrauber, *Software for the spectral analysis of scalar and vector functions on the sphere*, in Large Scale Scientific Computation, Academic Press, 1984.