PHYSICAL REVIEW D, VOLUME 62, 084026

Spectral methods for numerical relativity: The initial data problem

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(Received 2 November 1999; published 26 September 2000)

The partial differential equations of numerical relativity have traditionally been solved using a finite difference (FD) approximation. The accuracy of a FD solution increases as a fixed power of resolution while the computational resources required for the solution increase as the resolution raised to the (space + time) dimensionality of the problem. Modest accuracy solutions to problems involving either the initial conditions or the evolution of a dynamical black hole spacetime tax the capabilities of the computers presently available for the task, while the resources required for modest accuracy binary black hole problems are beyond what is presently available. For problems with smooth solutions alternatives to the FD approximation exist that may make more efficient use of the available computational resources. Here we investigate one of these techniques: the pseudo-spectral collocation (PSC) approximation. To determine its effectiveness relative to FD methods in solving problems in numerical relativity we use PSC to solve several two-dimensional problems that have been previously studied by other researchers using FD methods, focusing particularly on the computational resources required as a function of the desired solution accuracy. We find that PSC methods applied to these problems can achieve close to the theoretical limit of exponential convergence with problem resolution, while the computational resources required continue to scale only as the resolution raised to the problem dimensionality. Correspondingly, for solutions of even modest accuracy we find that PSC is substantially more efficient, as measured by either execution time or memory required, than FD; furthermore, these savings increase rapidly with increasing accuracy. We also discuss less quantitative but no less tangible advantages that the PSC approximation holds over the FD approximation. In particular, the solution provided by PSC is an analytic function given everywhere on the computational domain, not just at fixed grid points. Consequently, no *ad hoc* interpolation operators are required to determine field values at intermediate points or to evaluate the approximate solution or its derivatives on the boundaries. Since the practice of numerical relativity by finite differencing has been, and continues to be, hampered by both high computational resource demands and the difficulty of formulating acceptable finite difference alternatives to the analytic boundary conditions, we argue that PSC should be further pursued as an alternative way of formulating the computational problem of finding numerical solutions to the field equations of general relativity.

PACS number(s): 04.25.Dm, 02.70.Hm

I. INTRODUCTION AND SUMMARY

The partial differential equations (PDE) of numerical relativity have typically been solved using finite difference methods. In finite differencing (FD) one first chooses a finite number of coordinate ''grid'' points x_n and approximates the space and time derivatives in the PDEs by ratios of differences between field and coordinate values on the grid. With a choice of grid and ''differencing scheme'' for converting derivatives to ratios of differences, the equations of general relativity are approximated by a system of algebraic equations whose solution approximates that of the underlying PDEs.

In this paper we explore an alternative method for solving the elliptic PDEs encountered in numerical relativity: pseudo-spectral collocation (PSC). In PSC one begins by postulating an approximate solution, generally as a sum over some finite basis of polynomials or trigonometric functions. The coefficients in the sum are determined by requiring that the residual error, obtained by substituting the approximate solution into the exact PDEs, is minimized in some suitable sense. Thus, if one describes FD as finding the exact solution to an approximate system of equations, one can describe PSC as finding an approximate solution to the exact equations.

Pseudo-spectral collocation has been applied successfully to solve problems in many fields, including fluid dynamics, meteorology, seismology, and relativistic astrophysics (cf. [1–4]). Its advantage over FD arises for problems with smooth solutions, where the approximate solution obtained using PSC converges on the actual solution *exponentially* as the number of basis functions is increased. The approximate FD solution, on the other hand, never converges faster than algebraically with the number of grid points. While the computational cost per ''degree of freedom'' — basis functions for PSC, grid points for FD — is higher for PSC than for FD, the computational cost of a high accuracy PSC solution is a small fraction of the cost of an equivalent FD solution. Even for problems in which only modest accuracy is needed, PSC generally results in a significant computational savings in both memory and time compared to FD, especially for multidimensional problems.

The detailed relative performance of alternative solution techniques is necessarily problem, formulation and result specific. The asymptotic behavior of different solution methods can be revealing, but it is the real resources required for a solution of specified accuracy that is important to us. Here we investigate the relative performance of the FD and PSC approximations applied to several problems in numerical relativity. We focus on the solution of the elliptic constraint equations for two axisymmetric problems: the initial data for a black hole spacetime with angular momentum, and a spacetime with a black hole superposed with gravitational waves (Brill waves). We have chosen these problems because solutions in the FD approximation have been found for both by other researchers [5–7], and also the complexity of the spatial operators are representative of the more complex three-dimensional problems in numerical relativity, but not so complex that their formulation and solution obscures the nature of our investigation, which is the relative efficiency of the FD and PSC approximations to their solution.

In Sec. II we review briefly the key constraint equations that arise in the traditional space-plus-time decomposition of the Einstein field equations. (Experts may wish to skip this review, which is intended principally for the non-expert, and proceed directly to Sec. III where we describe the PSC approximation.) We describe three different elliptic problems: a nonlinear model problem whose analytic solution is known, the nonlinear Hamiltonian constraint equation for an axisymmetric black hole spacetime with angular momentum, and the Hamiltonian constraint equation for a spacetime with a black hole superposed with Brill waves. The solution to each of these problems using FD techniques has been reported on by other researchers; we use those solutions together with our own, obtained using the PSC approximation, to compare the efficiency of FD and PSC solution methods on representative problems in vacuum numerical relativity.

In Sec. III we describe in detail the PSC approximation, while in Sec. IV we compare the idealized asymptotic performance of PSC and FD solutions to problems with smooth solutions. In Sec. V we solve the problems described in Sec. II using PSC and compare the performance of these PSC solutions with the FD solutions to the same problems obtained by other authors. In Sec. VI, we discuss the results of our comparisons as well as other differences between PSC and FD techniques, and their implications for solving problems in vacuum numerical relativity. Finally, whether by FD or PSC the solution of the nonlinear elliptic systems described here involves solving a potentially large system of (nonlinear) algebraic equations. We describe the methods we use for solving them in Appendix A.

II. INITIAL VALUE EQUATIONS

A. Introduction

We use the standard 3+1 formalism of [8] which is discussed in detail by [9]. The general relativistic Cauchy initial value problem requires that we specify the metric γ_{ij} and extrinsic curvature K_{ij} of a three-dimensional spacelike hypersurface. These quantities cannot be specified arbitrarily: rather they must satisfy a set of constraint equations, which are a subset of the Einstein field equations. The four constraint equations (in vacuum) are

$$ {}^{(3)}R + K^2 - K_{ab}K^{ab} = 0, \tag{2.1a} $$

$$ {}^{(3)}\nabla_a (K^{ia} - K\gamma^{ia}) = 0, \tag{2.1b} $$

where ${}^{(3)}R$ is the Ricci scalar associated with γ_{ij}, ${}^{(3)}\nabla_a$ is the covariant derivative associated with γ_{ij}, and $K := K_{ab}\gamma^{ab}$.

York [9] has developed a convenient formalism for specifying the initial data such that Eqs. (2.1) are satisfied. Split γ_{ij} into a conformal factor ψ and the conformal metric $\overline{\gamma}_{ij} := \psi^{-4}\gamma_{ij}$, and K^{ij} into its trace K and its trace-free part $A^{ij} := K^{ij} - \frac{1}{3}\gamma^{ij}K$. The constraint equations (2.1) then become

$$ \overline{\nabla}^2\psi - \frac{1}{8}\overline{R}\psi - \frac{1}{12}K^2\psi^5 + \frac{1}{8}\overline{A}_{ab}\overline{A}^{ab}\psi^{-7} = 0, \tag{2.2a} $$

$$ \overline{\nabla}_a\overline{A}^{ia} - \frac{2}{3}\psi^6\overline{\gamma}^{ia}\overline{\nabla}_a K = 0, \tag{2.2b} $$

where ${}^{(3)}\overline{\nabla}_i$ is the covariant derivative and $\overline{R}$ is the Ricci scalar associated with $\overline{\gamma}_{ij}$, and $\overline{A}^{ij} := \psi^{10}A^{ij}$. Equation (2.2a) is generally referred to as the Hamiltonian constraint, while Eqs. (2.2b) are generally referred to as the momentum constraints. For the problems examined in this paper, the momentum constraints can be solved analytically. Therefore we will only need to apply our PSC method to solving the Hamiltonian constraint (2.2a) for the conformal factor ψ.

In order to solve the Hamiltonian constraint we must specify the boundary conditions. The problems we examine consist of an axisymmetric spacetime containing a single black hole. Let the initial hypersurface be asymptotically flat, so that on the hypersurface far from the black hole the curvature vanishes. Describe the black hole by an Einstein-Rosen bridge (i.e., by two asymptotically flat three-surfaces connected by a throat) and insist that the spacetime be inversion symmetric through the throat. These choices impose the boundary conditions

$$ \lim_{r\to\infty}\psi(r) = 1 \quad \text{asymptotic flatness}, \tag{2.3a} $$

$$ \left[\frac{\partial\psi}{\partial r} + \frac{\psi}{2a}\right]_{r=a} = 0 \quad \text{inversion symmetry}, \tag{2.3b} $$

$$ \left(\frac{\partial\psi}{\partial\theta}\right)_{\theta=0,\pi} = 0 \quad \text{axisymmetry}, \tag{2.3c} $$

on ψ where $r=a$ is the coordinate location of the throat.

A useful diagnostic of an initial data slice is to compute the total energy contained in the slice. Ó Murchadha and York [10] have examined the ADM energy (cf. [8]) in terms of the conformal decomposition formalism. For the problems we will examine below, the ADM energy is given by

$$ E_{ADM} = -\frac{1}{2\pi}\oint_\infty \overline{\nabla}^j\psi d^2\overline{S}_j, \tag{2.4} $$

i.e., it is proportional to the integral of the normal component of the gradient of the conformal factor about the sphere at infinity.

B. Three test problems

1. A model problem

Bowen and York [11] describe a nonlinear ''model'' of the Hamiltonian constraint equation that can be solved exactly, which we utilize in Sec. V to test our code. The model equation is

$$\overline{\nabla}^2\psi+\frac{3}{4}\frac{P^2}{r^4}\left(1-\frac{a^2}{r^2}\right)^2\psi^{-7}=0, \tag{2.5}$$

with P a constant. Together with the boundary conditions described above [Eqs. (2.3)], Eq. (2.5) has the solution

$$\psi=\left[1+\frac{2E}{r}+6\frac{a^2}{r^2}+\frac{2a^2E}{r^3}+\frac{a^4}{r^4}\right]^{1/4}, \tag{2.6a}$$

where

$$E=(P^2+4a^2)^{1/2}. \tag{2.6b}$$

If we evaluate Eq. (2.4) for this solution, we find that it has ADM energy E.

2. Black hole with angular momentum

Focus next on the initial data corresponding to an axisymmetric black hole spacetime with angular momentum. This problem was first examined analytically by [11], and has been explored numerically by [5,6]. Choosing the conformal background metric to be flat, [11] found an analytic solution to the momentum constraints (2.2b) that carries angular momentum and obeys the isometry condition at the black hole throat. Corresponding to this solution is the Hamiltonian constraint [Eq. (2.2a)] for the conformal factor ψ,

$$\overline{\nabla}^2\psi+\frac{9}{4}\frac{J^2\sin^2\theta}{r^6}\psi^{-7}=0, \tag{2.7}$$

where J is the angular momentum of the physical space.

3. Black hole plus Brill wave

The second physical problem upon which we demonstrate the use of spectral methods for numerical relativity is that of a black hole superposed with a Brill [12] wave, a problem studied using FD by [7]. Let the initial slice be a spacetime isometry surface (i.e., time symmetric); then, the extrinsic curvature K_{ij} vanishes and the momentum constraints [Eqs. (2.2b)] are trivially satisfied. Let the line-element of the conformal background metric have the form

$$\overline{ds^2}=[e^{2q}(dr^2+r^2d\theta^2)+r^2\sin^2\theta d\phi^2], \tag{2.8}$$

where

$$q:=A\sin^n\theta\left\{\exp\left[-\left(\frac{\eta+\eta_0}{\sigma}\right)^2\right]+\exp\left[-\left(\frac{\eta-\eta_0}{\sigma}\right)^2\right]\right\}, \tag{2.9}$$

$\eta:=\ln(r/a)$, n is an even integer, and A, η_0, and σ are constant parameters that describe the superposed Brill wave's amplitude, position, and width, respectively. With this choice the Hamiltonian constraint equation becomes

$$\frac{\partial^2\psi}{\partial r^2}+\frac{2}{r}\frac{\partial\psi}{\partial r}+\frac{1}{r^2}\frac{\partial^2\psi}{\partial\theta^2}+\frac{\cot\theta}{r^2}\frac{\partial\psi}{\partial\theta}+\frac{\psi}{4}\left(\frac{\partial^2 q}{\partial r^2}+\frac{1}{r}\frac{\partial q}{\partial r}+\frac{1}{r^2}\frac{\partial^2 q}{\partial\theta^2}\right)=0. \tag{2.10}$$

III. SPECTRAL METHODS

A. Introduction

Consider an elliptic differential equation, specified by the operator L on the d-dimensional open, simply-connected domain $\mathcal{D}$, with boundary conditions given by the operator S on the boundary $\partial\mathcal{D}$:

$$L(u)(\boldsymbol{x})=f(\boldsymbol{x}),\quad \boldsymbol{x}\in\mathcal{D}, \tag{3.1a}$$

$$S(u)(\boldsymbol{x})=g(\boldsymbol{x}),\quad \boldsymbol{x}\in\partial\mathcal{D}. \tag{3.1b}$$

There may be more than one boundary condition, in which case we can index S and g over the boundary conditions.

Approximate the solution $u(\boldsymbol{x})$ to this system as a sum over a sequence of *basis functions* $\phi_k(\boldsymbol{x})$ on $\mathcal{D}+\partial\mathcal{D}$,

$$u_N(\boldsymbol{x})=\sum_{k=0}^{N-1}\tilde{u}_k\phi_k(\boldsymbol{x}), \tag{3.2}$$

where the $\tilde{u}_k$ are constant coefficients. Corresponding to the approximate solution u_N is a residual R_N on $\mathcal{D}$ and r_N on $\partial\mathcal{D}$:

$$R_N=L(u_N)-f\quad\text{on}\quad\mathcal{D}, \tag{3.3a}$$

$$r_N=S(u_N)-g\quad\text{on}\quad\partial\mathcal{D}. \tag{3.3b}$$

The residual vanishes everywhere for the exact solution u.

In PSC we determine the coefficients $\tilde{u}_k$ by requiring that u_N satisfies the differential equation and boundary conditions *exactly* at a fixed set of *collocation points* x_n: i.e., we require that

$$0=L[u_N(x_n)]-f(x_n)\quad\text{for}\quad x_n\quad\text{in}\quad\mathcal{D}, \tag{3.4a}$$

$$0=S[u_N(x_n)]-g(x_n)\quad\text{for}\quad x_n\quad\text{on}\quad\partial\mathcal{D}, \tag{3.4b}$$

for all n. When the expansion functions and collocation points are chosen appropriately a numerical solution of these equations can be found very efficiently. In the following subsection we discuss choices of the expansion basis and collocation points.

B. Expansion basis and collocation points

In PSC we require that the approximate solution u_N satisfies the differential equation and boundary conditions exactly at the N collocation points x_n. The basis ϕ_k should not constrain the values of the approximation at the collocation points; correspondingly, we can write the basis as a set of N functions $\phi_k(x)$ that satisfy a discrete orthogonality relationship on the collocation points x_n:

$$\sum_{n=0}^{N-1} \phi_j(x_n)\phi_k^*(x_n)=\nu_k^2\delta_{jk}, \tag{3.5}$$

where the ν_k are normalization constants. Note that the basis functions are inextricably linked with the collocation points.

It is sometimes the case that the basis can be chosen so that the boundary conditions are automatically satisfied. For example, consider a one-dimensional problem on the interval

$$\mathbb{I}=[-1,1]. \tag{3.6}$$

If the boundary conditions are periodic then each element of the basis

$$\phi_k(x)=\exp[\pi i(x+1)k], \tag{3.7a}$$

satisfies the boundary conditions; correspondingly, the approximate solution u_N automatically satisfies the boundary conditions. If, in addition, we choose the collocation points

$$x_n=\frac{2n}{N}-1, \tag{3.7b}$$

then the basis satisfies the discrete orthogonality relation

$$\delta_{jk}=\frac{1}{N}\sum_{n=0}^{N-1} \phi_j(x_n)\phi_k^*(x_n). \tag{3.7c}$$

In an arbitrary basis, or with arbitrarily chosen collocation points, finding the $\tilde{u}_k$ from the $u_N(x_n)$ requires the solution of a general linear system of N equations in N unknowns, which involves $\mathcal{O}(N^3)$ operations. For the basis and collocation points given in Eqs. (3.7) the $\tilde{u}_k$ can be determined from the $u_N(x_n)$ quickly and efficiently via the fast Fourier transform in $\mathcal{O}(N\ln N)$ operations.

Arbitrary derivatives of the u_N can also be computed quickly: writing

$$\frac{d^p u_N}{dx^p}=\sum_{k=0}^{N-1} \tilde{u}_k^{(p)}\phi_k(x), \tag{3.8a}$$

we see immediately that

$$\tilde{u}_k^{(p)}=(\pi i k)^p\tilde{u}_k. \tag{3.8b}$$

Consequently, any derivative of u_N can be evaluated at all the collocation points in just $\mathcal{O}(N\ln N)$ operations.

The ability to evaluate efficiently the derivatives of u_N at the collocation points is much more important than finding a basis whose individual members satisfy the boundary conditions. In the case of periodic boundary conditions we can have our cake and eat it, too. More generally we choose a basis in which we can efficiently compute the derivatives of u_N at the collocation points and require separately that the approximate solution u_N satisfy the boundary conditions at collocation points on the boundary.

For general boundary conditions a basis of Chebyshev polynomials often meets all of our requirements.[1] Recall that the Chebyshev polynomials are defined on $\mathbb{I}$ by

$$T_k(x)=\cos(k\cos^{-1}x). \tag{3.9}$$

A simple recursion relation allows us to find the derivative of u_N as another sum over Chebyshev polynomials: if[2]

$$u_N(x)=\sum_{k=0}^{N} \tilde{u}_k T_k(x), \tag{3.10}$$

then

$$\frac{du_N}{dx}(x)=\sum_{k=0}^{N-1} \tilde{u}'_k T_k(x), \tag{3.11}$$

where

$$c_k\tilde{u}'_k=\tilde{u}'_{k+2}+2(k+1)\tilde{u}_{k+1}, \tag{3.12}$$

with

$$c_k=\begin{cases}2 & k=0,\\ 1 & k\geq 1.\end{cases} \tag{3.13}$$

If we choose collocation points x_n (for $0\leq n\leq N$) according to

$$x_n=\cos\frac{\pi n}{N}, \tag{3.14}$$

then the Chebyshev polynomials satisfy the discrete orthogonality relation

$$\delta_{jk}=\frac{2}{N\bar{c}_k}\sum_{n=0}^{N} \frac{1}{\bar{c}_n}T_j(x_n)T_k(x_n), \tag{3.15}$$

where

$$\bar{c}_k=\begin{cases}2 & k=0 \text{ or } N,\\ 1 & \text{otherwise.}\end{cases} \tag{3.16}$$

[1]The geometry of a problem might suggest other expansion functions, such as Legendre polynomials; however, a Chebyshev expansion does quite well and has the added convenience that, with appropriately chosen collocation points, only $\mathcal{O}(N\ln N)$ are required to convert from the expansion coefficients to the function values at the collocation points and vice versa [13].

[2]For Chebyshev bases the conventional notation is that k runs from 0 to N, not $N-1$; thus, there are $N+1$ coefficients and collocation points.

Finally, exploiting the relation between the Chebyshev polynomials and the Fourier basis [cf. Eq. (3.9)] allows us to find the $\tilde{u}_k$ from the $u_N(x_n)$ in $\mathcal{O}(N \ln N)$ time using a fast transform (see Appendix B of Ref. [2]). With an expansion basis of Chebyshev polynomials and an appropriate choice of collocation points we can thus evaluate derivatives of arbitrary order at the collocation points in $\mathcal{O}(N \ln N)$ operations.

For problems on an arbitrary domain of dimension d greater than unity it is rarely the case that we can find a basis which permits rapid evaluation of derivatives. Consider, however, a d-dimensional domain

$$\mathbb{D} = [a_1,b_1] \times [a_2,b_2] \times \cdots \times [a_d,b_d], \tag{3.17}$$

where $\{a_i\}$ and $\{b_i\}$ are constants. If the physical domain can be mapped smoothly to $\mathbb{D}$, then we can write

$$u_{N^{(1)} \ldots N^{(d)}}(\boldsymbol{x}) = \sum_{k_1=0}^{N^{(1)}} \cdots \sum_{k_d=0}^{N^{(d)}} \tilde{u}_{k_1 \cdots k_d} \phi_{k_1 \cdots k_d}(\boldsymbol{x}), \tag{3.18a}$$

where

$$\boldsymbol{x} = (x^{(1)}, \ldots, x^{(d)}), \tag{3.18b}$$

and $\phi_{k_1 \cdots k_d}$ is a tensor product of basis functions defined on one (e.g., Chebyshev polynomials) or more (e.g., spherical harmonics) dimensions. For example, if $\mathbb{D} = \mathbb{I}^d$, then we could choose

$$\phi_{k_1 \cdots k_d}(\boldsymbol{x}) = \prod_{l=1}^{d} \phi_{k_l}^{(l)}(x^{(l)}), \tag{3.18c}$$

where the $\{\phi_{k_l}^{(l)}\}$, for fixed l, is a basis on $\mathbb{I}$ which permits fast evaluation of derivatives with respect to its argument (e.g., Chebyshev polynomials).

Associated with each set of basis functions are the collocation points $x_n^{(l)}$; correspondingly, the collocation points associated with $\phi_{k_1 \cdots k_d}$ are just the $N_1 \cdots N_d$-tuples

$$\boldsymbol{x}_{n_1 \cdots n_d} = (x_{n_1}^{(1)}, \cdots, x_{n_d}^{(d)}). \tag{3.18d}$$

With this choice of basis and collocation points we can evaluate efficiently arbitrary derivatives of an approximation $u_{N^{(1)} \ldots N^{(d)}}$. If the domain cannot be mapped smoothly to $\mathbb{D}$, either more sophisticated methods such as domain decomposition [1,2] must be used, or the problem may not be amenable to solution by PSC. See [14] for an example of using multiple spherical-like domains for astrophysical problems.

C. Solving the system of equations

The expansion basis, collocation points and differential equation with boundary conditions determine a system of equations for the coefficients $\tilde{u}_k$ or, equivalently, the approximate solution u_N evaluated at the collocation points. Iterative solution methods [which require as few as $\mathcal{O}(N \ln N)$ operations] work well to solve the kind of systems of equations that arise from the application of a PSC method.

If the elliptic system being solved is linear then the algebraic equations arising from either a FD or a PSC method are also linear and a unique solution is guaranteed. If, on the other hand, the differential system is nonlinear, then the equations arising from FD or PSC are also nonlinear and a unique solution is not guaranteed. Newton's method (see Sec. 12.13 and Appendices C and D of Ref. [1]), where one solves the linearized equations beginning with a guess and then iterating, works well for these types of equations. As long as a good initial guess is chosen, the iteration will usually converge. In Appendix A we describe in detail the variant of Newton's method (Richardson's iteration) that we have used to solve the nonlinear system of algebraic equations that arise when we apply PSC to solve the Hamiltonian constraint equations as posed in Sec. II.

IV. COMPARING FINITE DIFFERENCE AND PSEUDO-SPECTRAL COLLOCATION METHODS

A. Introduction

Finite differencing and pseudo-spectral collocation are alternative ways to find approximate solutions to a system of differential equations. Consider the Poisson problem in one dimension:

$$\frac{d^2u}{dx^2} = f(x), \tag{4.1a}$$

on the interval $\mathbb{I}$ with Dirichlet boundary conditions

$$u(-1) = u(1) = 0. \tag{4.1b}$$

In a FD approach to this problem we seek the values of u at discrete points x_n, say

$$x_n = -1 + \frac{2n}{N}, \tag{4.2}$$

for $n = 0,1, \ldots, N$. Algebraic equations are found by approximating the differential operator d^2u/dx^2 in Eq. (4.1a) by a ratio of differences: e.g.,

$$\frac{d^2u}{dx^2}(x_n) \simeq \frac{u_{n+1} - 2u_n + u_{n-1}}{\Delta x^2}, \tag{4.3}$$

for integer $n = 1,2, \ldots N-1$ where

$$u_n := u(x_n), \tag{4.4a}$$

$$\Delta x := 2/N. \tag{4.4b}$$

With this discretization the differential equation (4.1a) yields $N-1$ equations for the $N+1$ unknown u_n. The boundary conditions [Eq. (4.1b)] yield two more equations, completely determining the u_n:

$$\frac{u_{n+1}-2u_n+u_{n-1}}{\Delta x^2}=f(x_n), \quad 1\leqslant n\leqslant N-1, \tag{4.5a}$$

$$u_0=0, \tag{4.5b}$$

$$u_N=0. \tag{4.5c}$$

The solution to these equations is the FD approximation to $u(x)$ at the points x_n.

The FD solution to Eqs. (4.1) begins by approximating the differential equations. In the PSC method, on the other hand, we first approximate the solution at all points in $\mathbb{I}$ by a sum over a finite set of basis functions. For this example, we choose a Chebyshev basis; so, we write

$$u_N(x)=\sum_{k=0}^{N}\tilde{u}_k T_k(x). \tag{4.6}$$

Now insist that u_N satisfies the differential equation and boundary conditions exactly at the collocation points

$$x_n=\cos\frac{\pi n}{N}, \tag{4.7}$$

for $n=0,1,\ldots N$. In particular, we require that the boundary conditions are satisfied and that, in addition, the differential equation is satisfied for integer n ranging from 1 to $N-1$:

$$u_N(x_0)=0, \tag{4.8a}$$

$$u_N(x_N)=0, \tag{4.8b}$$

$$\frac{d^2u_N}{dx^2}(x_n)=f(x_n). \tag{4.8c}$$

To evaluate Eq. (4.8c) note that d^2u_N/dx^2 can be written as

$$\frac{d^2u_N}{dx^2}(x_n)=\sum_{m=0}^{N} d^{(2)}_{nm}u_N(x_m). \tag{4.9a}$$

The $d^{(2)}_{nm}$ can be determined by noting that

$$\frac{d^2u_N}{dx^2}(x_n)=\sum_{k=0}^{N}\tilde{u}''_k T_k(x_n), \tag{4.9b}$$

with

$$c_k\tilde{u}''_k=\tilde{u}''_{k+2}+2(k+1)\tilde{u}'_{k+1},$$

$$c_k\tilde{u}'_k=\tilde{u}'_{k+2}+2(k+1)\tilde{u}_{k+1}, \tag{4.9c}$$

and

$$\tilde{u}_k=\frac{2}{N\bar{c}_k}\sum_{n=0}^{N}\frac{1}{\bar{c}_n}u_N(x_n)T_k(x_n), \tag{4.9d}$$

where c_k and $\bar{c}_k$ are given by Eqs. (3.13) and (3.16), respectively.

The result is, again, a set of algebraic equations for $u_N(x_n)$: the values of the approximate solution at the collocation points. Finding the $u_N(x_n)$ yields an approximate solution to the differential equation over the entire domain $\mathbb{I}$ since the spectral coefficients $\tilde{u}_k$ are given by Eq. (4.9d).[3]

For the linear problem posed here the solution to the algebraic system of equations that arise in either a FD or PSC solution can be solved directly or by any of the many standard iterative methods. For nonlinear problems the systems are generally solved by linearizing the equations about an initial guess and then iterating the solution until it converges. We discuss one method of solution in Appendix A.

B. Convergence of approximations

In either a FD or PSC solution to a differential equation with boundary conditions we expect that, as N tends to infinity, the approximate solution should become arbitrarily accurate. For large N, the L_2 error in a FD approximation converges upon the exact solution as N^{-p} for positive integer p. The value of p depends on the smoothness of f and the error in the approximation of the differential operator (in the example above, d^2/dx^2). Assuming that f is smooth the rate of convergence (measured by the L_2 error of the FD solution) is N^{-p} when the truncation error of the differential operator is $\mathcal{O}(\Delta x^p)$.

In contrast, when the solution u is smooth the error made by a properly formulated spectral approximation decreases faster than any fixed power of N (where N is now the number of collocation points or basis functions).[4] For a heuristic understanding of this rapid convergence, note first that a PSC solution's derivatives at each collocation point involve all the $\{u_N(x_n)\}$ [cf. Eq. (4.9)]. Correspondingly, it is as exact as possible, given the information available at the N collocation points. This suggests that an order N collocation spectral approximation to the derivatives of the unknown should make errors on order $\mathcal{O}(\Delta x^N)$. The interval Δx, however, is also proportional to N^{-1}; so, we expect that the error in the spectral solution u_N should vary as $\mathcal{O}(N^{-N})$. A more rigorous analysis using convergence theory (see Chap. 2 of Ref. [1]), shows that for any function which is analytic on the domain of interest, a Chebyshev expansion will converge exponentially [i.e. as $\mathcal{O}(e^{-N})$]. If the function is also periodic then a Fourier expansion will converge exponentially.

C. Computational cost of solutions

The computational cost, in time, of a FD solution to a system of elliptic differential equations scales linearly with the number of grid points N while the accuracy ϵ of the solution scales as N^{-p}, where p is the order of the FD operator truncation error. Correspondingly, the cost $K_{\rm FD}$ for a given accuracy scales as

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[3]Alternatively, we could have constructed a system of equations in terms of the unknown spectral coefficients. This would correspond to a spectral tau method: cf. [1,2].

[4]In addition the individual spectral coefficient $\tilde{u}_k$ should decrease exponentially with N once the problem is sufficiently resolved.

$$K_{\rm FD} \sim \epsilon^{-1/p}. \tag{4.10a}$$

The cost $K_{\rm PSC}$ of a PSC solution to the same system, on the other hand, scales as $N \ln N$ (for an iterative solution) while ϵ scales as $\exp(-N)$; consequently, the cost scales with accuracy ϵ as

$$K_{\rm PSC} \sim -(\ln \epsilon)\ln(-\ln \epsilon). \tag{4.10b}$$

Since it is the computational cost required to achieve a given accuracy that is important, the more rapid convergence of a PSC solution confers upon it a clear advantage. This advantage is made clear by considering how the ratio of costs scales with accuracy:

$$\frac{K_{\rm PSC}}{K_{\rm FD}} \sim -\epsilon^{1/p} \ln \epsilon \ln(-\ln \epsilon), \tag{4.11}$$

which tends to zero with ϵ; consequently, increasing accuracy with a PSC solution is always more efficient than with a FD solution.

The equations that arise from either a FD or PSC treatment of an elliptic differential system are typically solved using iterative methods; thus, *at fixed resolution* the storage requirements for either solution method are equivalent. As we have seen, however, fixed resolution does not correspond to fixed solution accuracy. As the desired solution accuracy increases, the storage requirements of a PSC solution fall relative to those of an FD solution by a factor of $-\epsilon^{1/p}\ln \epsilon$.

V. SOLVING THE HAMILTONIAN CONSTRAINT

A. Nonlinear model problem

As a first example we solve the model Hamiltonian constraint equation (2.5) described in Sec. II B 1, with the boundary conditions (2.3) on the domain $r \in [a,\infty)$. As described this problem is spherically symmetric; nevertheless, we treat it as axisymmetric to illustrate the methods used to solve the Hamiltonian constraint for the black hole with angular momentum (cf. Sec. II B 2) and the black hole plus Brill wave problems (cf. Sec. II B 3).

As a first step we map the domain $r \in [a,\infty), \theta \in [0,\pi]$ to a square in $\mathbb{R}^2$: letting

$$x = \frac{2a}{r} - 1, \tag{5.1a}$$

$$y = \cos\theta, \tag{5.1b}$$

we have $x \in (-1,1]$ and $y \in [-1,1]$. In terms of the (x,y) coordinates, the model Hamiltonian constraint [Eq. (2.5)] becomes

$$(x+1)^2 \frac{\partial^2 \psi}{\partial x^2} + (1-y^2)\frac{\partial^2 \psi}{\partial y^2} - 2y\frac{\partial \psi}{\partial y} + \frac{3}{256}\left(\frac{P}{a}\right)^2 (x+1)^2(3-2x-x^2)^2\psi^{-7} = 0, \tag{5.2}$$

subject to the boundary conditions

$$\lim_{x\to -1} \psi = 1, \tag{5.3a}$$

$$\left[\frac{\partial \psi}{\partial x} - \frac{1}{4}\psi\right]_{x=1} = 0. \tag{5.3b}$$

Note that with our choice of variables and expansion bases the angular boundary conditions [Eq. (2.3c)] are automatically satisfied.

Since ψ is not periodic in either x or y, we adopt a Chebyshev basis for the approximate solution:

$$\psi_{N_x,N_Y}(x,y) = \sum_{j=0}^{N_x}\sum_{k=0}^{N_y} \tilde{\psi}_{jk} T_j(x) T_k(y), \tag{5.4a}$$

with the corresponding collocation points

$$x_j = \cos\frac{\pi j}{N_x}, \tag{5.4b}$$

$$y_k = \cos\frac{\pi k}{N_y}. \tag{5.4c}$$

For this problem, focus on approximations

$$\Psi_l = \psi_{4l,4}, \tag{5.5}$$

for integer l. We keep N_y fixed as the model problem is independent of y.

Following the discussion in Appendix A, solve the PSC equations using Richardson's iteration with a second-order FD preconditioner. To obtain Ψ_l, we need an initial guess $\Psi_l^{(0)}$ to begin the iteration. For the lowest resolution expansion $(N_x = 4)$ begin the iteration with the guess

$$\Psi_1^{(0)}(x,y) = \frac{(3+x)}{2}, \tag{5.6}$$

which is the trivial solution for $P=0$. Applying Richardson's iteration will then give us the approximate solution Ψ_1. Through the expansion (5.4a) this determines an approximation for ψ everywhere; in particular, it determines an approximation at the collocation points corresponding to $N_x = 8$, which we then use as the initial guess for determining the approximate solution Ψ_2. In this same way we use a lower-resolution approximate solution as the initial guess for the approximate solution at the next higher-resolution, i.e.

$$\Psi_l^{(0)} = \Psi_{l-1}. \tag{5.7}$$

To investigate the accuracy of our solution as a function of resolution (basis dimension for PSC, number of grid points for FD) we evaluate a number of solutions differing only in resolution and evaluate several different error measures.

(1) For this problem we know the exact solution [cf. Eq. (2.6)]; so, we calculate the L_2 norm of the absolute error as a function of l:

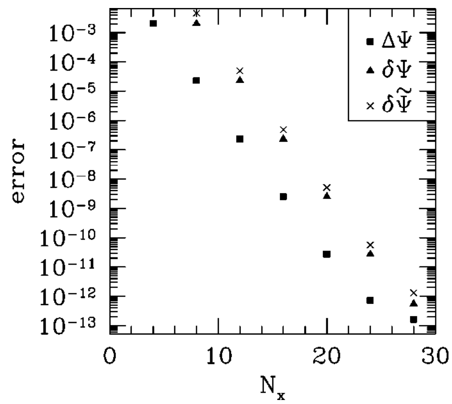

FIG. 1. Spectral convergence for a nonlinear model problem. Plotted are a measure of the absolute error $\Delta\Psi_l$, and two approximate measures of the error $\delta\Psi_l$ and $\delta\tilde{\Psi}_l$ as a function of N_x, the number of radial functions, for the case $P=1$.

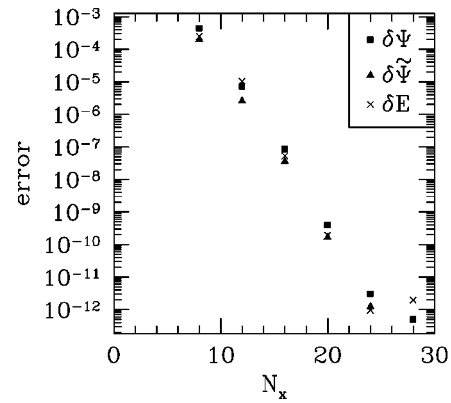

FIG. 2. Spectral convergence for the solution of the Hamiltonian constraint equation for a black hole with angular momentum. Plotted are three approximate measures of the error $\delta\Psi_l$, $\delta\tilde{\Psi}_l$ and δE as a function of N_x, the number of radial functions, for $J=1$.

$$\Delta\Psi_l=\left\{\sum_{j=0}^{N_x}\sum_{k=0}^{N_y}\frac{1}{N_xN_y\overline{c_jc_k}}[\Psi_l(x_j,x_k)-\psi(x_j,x_k)]^2\right\}^{1/2} :=\|\Psi_l-\psi\|_2, \tag{5.8}$$

where c_k is given by Eq. (3.16).

(2) We can also characterize the convergence of the approximate solutions Ψ_l by calculating the L_2 norm of the difference between the successive approximate solutions:

$$\delta\Psi_l=\|\Psi_l-\Psi_{l-1}\|_2. \tag{5.9}$$

The errors $\delta\Psi$ and $\Delta\Psi$ are defined for either FD or PSC solutions.

(3) We also evaluate, by analogy with $\Delta\Psi$ and $\delta\Psi$, the quantities

$$\Delta E_l=|E_l-E|, \tag{5.10}$$

$$\delta E_l=|E_l-E_{l-1}|, \tag{5.11}$$

where E_l is the ADM mass-energy associated with the approximate conformal factor Ψ_l. We evaluate E using Eq. (2.4).

(4) For PSC solutions only we define the relative error measure

$$\delta\tilde{\Psi}_l=\sum_{j=0}^{N_x}\sum_{k=0}^{N_y}|\tilde{\psi}_{jk}^{(l)}-\tilde{\psi}_{jk}^{(l-1)}|, \tag{5.12}$$

which characterizes the changes in the spectral coefficients as the order of the approximation increases.

For a properly formulated spectral method, all of our error measures should decrease exponentially with N if the solution to the problem is analytic.

Figure 1 shows the absolute and relative errors $\Delta\Psi_l$ and $\delta\Psi_l$, along with the change in the spectral coefficients $\delta\tilde{\Psi}_l$, for $P=1$. The exponential convergence of the solution with increasing N_x is apparent. Experience shows that as the problem becomes more nonlinear (i.e., P becomes larger) more terms are needed in the expansion in order to achieve the same accuracy.

This system of equations has also been solved using FD methods [6]. A point comparison is telling: in [6] a second order accurate FD solution with a resolution of 1024 radial points were required for a solution with a $\Delta E\simeq10^{-5}$, independent of P. The PSC solution described here achieves the same accuracy using an expansion with only 12 radial functions for $P=1$, and 24 functions for $P=10$. In either case a PSC solution with an accuracy of $\Delta E\approx10^{-10}$ is obtained by doubling the number of radial functions. To achieve the same accuracy the FD approximation would require (assuming second order FD) a resolution of 3×10^5 radial points.

B. Black hole with angular momentum

Now turn to consider a truly non-radial, but still axisymmetric, problem: a rotating black hole (cf. Sec. II B 2). As before [cf. Eq. (5.1)] we map the semi-infinite domain $r\geqslant a$ to the finite box $x\in(-1,1]$, $y\in[-1,1]$, obtaining the system of equations

$$(x+1)^2\frac{\partial^2\psi}{\partial x^2}+(1-y^2)\frac{\partial^2\psi}{\partial y^2}-2y\frac{\partial\psi}{\partial y} +\frac{9}{64}\left(\frac{J}{a^2}\right)^2(x+1)^4(1-y^2)\psi^{-7}=0, \tag{5.13}$$

subject to the boundary conditions given in Eqs. (5.3).

For this problem we do not have the exact solution; so, we consider only the relative errors $\delta\Psi$, $\delta\tilde{\Psi}$ and δE. Figure 2 (3) shows these quantities as functions of N_x for J/M^2 equal to 1 (100). For these solutions $\Psi_l=\psi_{4l,N_y}$, where initially $N_y=4$ and is incremented by two[5] whenever the difference

[5]Along with axisymmetry, this problem has equatorial plane symmetry so Ψ_l is even in y. By exploiting this symmetry, we could reduce our number of angular functions by a factor of two.

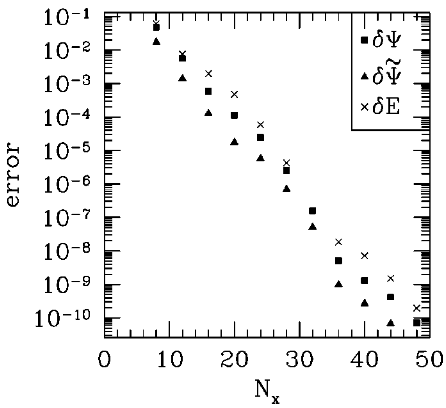

FIG. 3. Same as Fig. 2 with $J=100$.

between $\delta\Psi_l$ with and without the increment was greater than ten percent. Again we see rapid, exponential convergence of the solution with N.

This problem has also been solved using second order FD [6]. For a solution accuracy $\delta E \simeq 10^{-5}$, [6] found that a resolution 1024 radial and 384 angular grid points was required, roughly independent of the value of J. We find that PSC achieves the same accuracy with an expansion basis of 12 radial (and 4 angular) functions for $J=1$, and 24 radial (and 8 angular) functions for $J=100$. Solution accuracies of 10^{-10} can be obtained for the PSC solution simply by doubling the size of the expansion basis (in x and y). For a similar increase in accuracy of the FD solution a grid approximately 300 times larger in each dimension would be required.

C. Black hole plus Brill wave

As a final example we consider the Hamiltonian constraint for a black hole superposed with a Brill wave. After mapping this problem to the (x,y) domain we obtain the system of equations

$$(x+1)^2\frac{\partial^2\Psi}{\partial x^2}+(1-y^2)\frac{\partial^2\Psi}{\partial y^2}-2y\frac{\partial\Psi}{\partial y}+\frac{\Psi R}{4}=0, \tag{5.14a}$$

with

$$R=(x+1)^2\frac{\partial^2 q}{\partial x^2}+(x+1)\frac{\partial q}{\partial x}+(1-y^2)\frac{\partial^2 q}{\partial y^2}-y\frac{\partial q}{\partial y}, \tag{5.14b}$$

where q is given by Eq. (2.9), and subject to the boundary conditions (5.3).

In Fig. 4 we show $\delta\tilde{\Psi}$ as a function of N_x for the Brill wave parameters $\sigma=A=\eta_0=1$ and $n=2$. For these solutions $\Psi_l=\psi_{4l,N_y}$ where initially $N_y=4$, and is incremented by two whenever the difference between $\delta\Psi_l$ with and without the increment was greater than ten percent. The convergence, while rapid, is not quite exponential. In addition, the nearly exponentially decreasing error is impressed with a wave that is nearly periodic in spectral resolution $\log N_x$. We

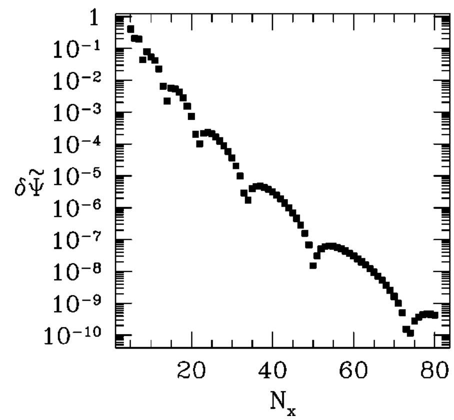

FIG. 4. Spectral convergence for the solution of the Hamiltonian constraint equation for a black hole plus Brill wave. Plotted is an approximate measure of the error $\delta\tilde{\Psi}_l$ as a function of N_x, the number of radial functions, for the case $A=\eta_0=\sigma=1$, $n=2$.

attribute this behavior to the resolution of the factor R [cf. Eq. (5.14b) and also Eq. (2.9) for q]. Figure 5 shows the error ΔR obtained when we form approximate R_{N_x,N_y} according to

$$R_{N_x,N_y}=\sum_{j=0}^{N_x}\sum_{k=0}^{N_y}\tilde{R}_{jk}T_j(x)T_j(y), \tag{5.15a}$$

$$\tilde{R}_{jk}=\frac{4}{N_xN_y\bar{c}_k\bar{c}_j}\sum_{l=0}^{N_x}\sum_{m=0}^{N_y}\frac{1}{\bar{c}_l\bar{c}_m}T_j(x_l)T_k(y_m)R(x_l,y_m). \tag{5.15b}$$

The structure in the solution is the same as the structure in the Chebyshev approximation to R.

This problem has also been solved using FD methods [7], enabling us to compare the resolution required for approximate FD or PSC solution for a given accuracy. With second order FD a solution whose error δE is 3×10^{-5} required a resolution of 400 radial and 105 angular grid points. To

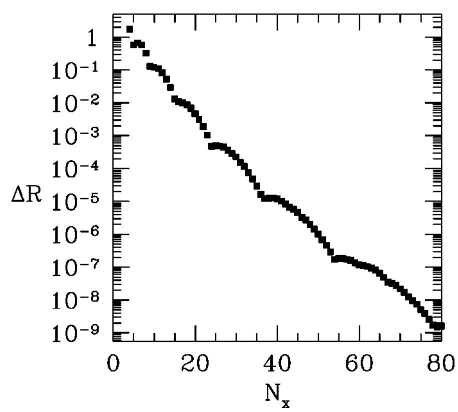

FIG. 5. The error in the spectral representation of R [Eq. (5.14b)] for the case shown in Fig. 4.

achieve the same accuracy the PSC solution described here requires a basis of only 36 radial (and 12 angular) Chebyshev polynomials.

VI. DISCUSSION

Pseudo-spectral collocation (PSC) is a very efficient way of solving the nonlinear elliptic equations that arise in numerical relativity. These problems typically have smooth solutions; correspondingly, the approximate solutions obtained using PSC converge upon the exact solution exponentially with the number of collocation points. As a result, the cost of a high accuracy PSC solution is not significantly greater than the cost of a similar solution of modest accuracy. Since the computational burden of solving the PSC equations with a given number of collocation points is no greater than that required to solve the finite difference equations for the same number of grid points, the computational demands of a PSC solution are far less than those of a finite difference solution for even modest accuracy.

While we have considered only axisymmetric problems in this paper, we have full confidence that PSC will perform just as well when applied to truly three-dimensional problems. In fact, [4,14] have applied spectral methods to numerous 3D problems in relativistic astrophysics with great success. In addition to our own work several other groups have applied PSC methods to problems in vacuum relativity. For example, [15] to compute initial data for the conformal Einstein's equations, [16] to evolve Einstein's equations in the null quasi-spherical gauge, and [17] to compute a shift vector for a Kerr black hole.

Numerical relativity research has developed the reputation that it can only be practiced by large groups using the most advanced computing hardware, and that progress is only possible through advances in computing hardware. It is certainly true that advances in hardware have and will continue to power advances in numerical relativity. Nevertheless, we maintain that there is room for substantially greater efficiency in the numerical methods employed and that the efficiency of PSC makes research addressing a wider range of significant problems possible sooner, and also accessible to smaller groups or individual investigators using local computing resources.

There is another important advantage of the PSC approximation, involving the formulation of boundary conditions, which has not so far been discussed. In a FD solution boundary conditions involving derivatives of the fields must be reformulated as finite difference equations. This generally involves the introduction of auxiliary boundary conditions, which are not part of the original problem. For example, consider the second order elliptic equation on $\mathbb{I}$:

$$\frac{d^2u}{dx^2}=f(x), \tag{6.1a}$$

$$u(-1)=u(1)=0. \tag{6.1b}$$

A fourth-order accurate finite difference approximation to the differential operator d^2/dx^2 is

$$\frac{16(u_{j-1}-2u_j+u_{j+1})-(u_{j-2}-2u_j+u_{j+2})}{\Delta x^2}=f(x_j), \tag{6.2}$$

where

$$u_j=u(j\Delta x). \tag{6.3}$$

Before this finite difference operator can be used in Eq. (6.1) it must be modified at the grid points $-1+\Delta x$ and $1-\Delta x$ since $-1-\Delta x$ and $1+\Delta x$ both lie outside the computational domain. In this case, four boundary conditions are required (at x equal to $-1,\ -1+\Delta x,\ 1-\Delta x$ and 1) even though the second order equation (6.1a) properly admits of only two boundary conditions.

In PSC, on the other hand, no auxiliary boundary conditions need be formulated. Since the approximate solution is expressed as an analytic function its derivatives on the boundary are known and can be required to satisfy the boundary condition equations exactly at the boundary collocation points.

These advantages of PSC solution come at a cost. When properly implemented the computational expense of PSC may be considerably less than the expense of finite differencing; however, the difficulty of implementation is greater. The efficient solution of the algebraic equations arising from PSC generally require the use of sophisticated iterative methods. Additionally, the exact solution itself must be smooth on the computational domain if the superior convergence of the solution is to be achieved. Finally, and perhaps most importantly, for problems of dimension greater than unity the computational domain must be sufficiently simple that it can be mapped to $\mathbb{D}$ (3.17) or be decomposed into sub-domains that can each be mapped to $\mathbb{D}$ (e.g., an L-shaped region can be decomposed into two regions, each of which can be mapped to $\mathbb{I}^2$). A spacetime containing multiple black holes cannot be mapped into $\mathbb{D}$. We believe, however, that such a spacetime can be treated using a multidomain PSC method. This is currently under investigation.

We have not here investigated the application of PSC techniques to evolution problems. PSC methods have been used to solve problems in other fields (e.g., fluid dynamics) with great success [2,18]. Our own experience in applying these techniques to 1D evolution problems in numerical relativity [19] shows promise, but our extension to evolution problems in multiple dimensions is not yet complete.

ACKNOWLEDGMENTS

It is a pleasure to acknowledge the support of the National Science Foundation (PHY/ASC93-18152, ARPA supplemented, PHY 98-00111, PHY 99-96213, PHY 95-03084, PHY 99-00672, PHY 94-08378). L.S.F. would also like to acknowledge the support of the Alfred P. Sloan Foundation.

APPENDIX A: SOLVING THE PSEUDO-SPECTRAL COLLOCATION EQUATIONS

In this appendix we describe one method of solving the nonlinear equations that arise from applying a PSC method to a nonlinear elliptic system of equations

$$L(u)=f \quad \text{on} \quad \mathcal{D}, \tag{A1a}$$

$$S(u)=g \quad \text{on} \quad \partial\mathcal{D}. \tag{A1b}$$

Choosing an expansion basis and corresponding collocation points, the PSC solution of these equations is fully characterized by the values of u_N at the collocation points x_n: from these the coefficients of the expansion and all the derivatives of the approximate solution can be determined. Write the values of the approximate solution u_N at the collocation points x_n as a vector $\boldsymbol{U}$,

$$\boldsymbol{U}_n=u_N(x_n). \tag{A2}$$

Corresponding to the approximate solution u_N is a *residual* R_N on $\mathcal{D}$ and r_N on $\partial\mathcal{D}$:

$$R_N=L(u_N)-f \quad \text{on} \quad \mathcal{D}, \tag{A3a}$$

$$r_N=S(u_N)-g \quad \text{on} \quad \partial\mathcal{D}. \tag{A3b}$$

The residual vanishes everywhere for the exact solution u. Write the values of the residual at the collocation points x_n as a vector $\boldsymbol{R}$,

$$\boldsymbol{R}_n=\begin{cases} R_N(x_n) & x_n \text{ on } \mathcal{D} \\ r_N(x_n) & x_n \text{ on } \partial\mathcal{D}. \end{cases} \tag{A4}$$

The PSC solution $\boldsymbol{U}$ satisfies the algebraic equations

$$\boldsymbol{R}[\boldsymbol{U}]=0. \tag{A5}$$

Before describing how to solve Eq. (A5) for a nonlinear system (i.e., nonlinear L or S) we describe the method of solution for a linear system.

When the system of differential equations (A1) is linear so is the system of algebraic equations (A5). In this case we can write

$$\boldsymbol{\Lambda}\boldsymbol{U}=\boldsymbol{F}, \tag{A6}$$

where $\boldsymbol{\Lambda}$ is a matrix and $\boldsymbol{F}$ is a vector whose components take on the values of f and g evaluated at the collocation points in the domain $\mathcal{D}$ and its boundary $\partial\mathcal{D}$. In PSC the matrix $\boldsymbol{\Lambda}$ is typically full. Direct solution methods require $\mathcal{O}(N^3)$ operations for such systems; for efficiency such systems are generally solved by iterative methods, which typically requires many fewer operations to find an accurate solution.

A simple and effective iterative method for solving Eq. (A6) is Richardson's iteration. Suppose we have a guess $\boldsymbol{V}^{(i)}$ to the solution $\boldsymbol{U}$ of Eq. (A6). A better approximation to $\boldsymbol{U}$ is $\boldsymbol{V}^{(i+1)}$ given by

$$\boldsymbol{V}^{(i+1)}=\boldsymbol{V}^{(i)}-\omega\boldsymbol{R}^{(i)}, \tag{A7}$$

where the residual $\boldsymbol{R}^{(i)}$ vector is given by

$$\boldsymbol{R}^{(i)}=\boldsymbol{\Lambda}\boldsymbol{V}^{(i)}-\boldsymbol{F}, \tag{A8}$$

and ω is a relaxation parameter, which must be determined. The optimal value of ω and the rate of convergence of the iterations depend upon the eigenvalues of $\boldsymbol{\Lambda}$. For Richardson's iteration the optimal ω is

$$\omega_{\text{opt}}=\frac{2}{\lambda_{\max}+\lambda_{\min}}, \tag{A9}$$

where $\lambda_{\max}$ and $\lambda_{\min}$ are the largest and smallest eigenvalues of $\boldsymbol{\Lambda}$. This choice minimizes the spectral radius ρ,

$$\rho=\frac{\lambda_{\max}-\lambda_{\min}}{\lambda_{\max}+\lambda_{\min}}, \tag{A10}$$

of the iteration matrix, $G=I-\omega\Lambda$. The convergence rate of the iteration is [2]

$$\mathcal{R}=-\ln\rho. \tag{A11}$$

The reciprocal of $\mathcal{R}$ measures the number of iterations required to reduce the error by a factor of e.

Richardson's iteration is, by itself, not necessarily more efficient than a direct solution method. Consider, for example, the second-order differential equation

$$\frac{d^2u}{dx^2}=f(x), \quad x\in(-1,1), \tag{A12a}$$

$$u(-1)=u(1)=0 \tag{A12b}$$

(cf. also Sec. IV). A PSC solution with a Chebyshev expansion basis leads to an operator $\boldsymbol{\Lambda}$ with a spectral condition number $\lambda_{\max}/\lambda_{\min}$ that is $\mathcal{O}(N^2)$. This gives a rate of convergence $\mathcal{R}\sim\mathcal{O}(N^{-2})$; correspondingly, $\mathcal{O}(N^2)$ iterations are required to obtain a reasonable solution. Since each iteration requires $\mathcal{O}(N\ln N)$ operations [i.e., it is asymptotically dominated by the cost of evaluating the derivatives d^2u/dx^2 given the $N+1$ $u_N(x_n)$] the total cost of obtaining a solution $\boldsymbol{U}$ is $\mathcal{O}(N^3\ln N)$, which is slightly *more* expensive than a direct solution.

We can speed the convergence of Richardson's iteration by solving an equivalent problem whose spectral condition number is better behaved. Introduce the *preconditioning* matrix $\boldsymbol{H}$ and consider the equivalent system

$$\boldsymbol{H}^{-1}\boldsymbol{\Lambda}\boldsymbol{U}=\boldsymbol{H}^{-1}\boldsymbol{F}. \tag{A13}$$

Now given an approximation $\boldsymbol{V}^{(i)}$ to $\boldsymbol{U}$, a better approximation $\boldsymbol{V}^{(i+1)}$ is given by

$$\boldsymbol{V}^{(i+1)}=\boldsymbol{V}^{(i)}-\omega'\boldsymbol{H}^{-1}\boldsymbol{R}^{(i)}, \tag{A14}$$

where $\boldsymbol{R}^{(i)}$ is given as before and ω' is related to the eigenvalues of the linear operator $\boldsymbol{H}^{-1}\boldsymbol{\Lambda}$.

In practice we never actually invert the preconditioning matrix H; instead we solve

$$\boldsymbol{H}(\boldsymbol{V}^{(i+1)}-\boldsymbol{V}^{(i)})=-\omega'\boldsymbol{R}^{(i)}, \tag{A15}$$

for successive approximations. In order that this equation for successive approximations should converge rapidly we require a preconditioning matrix $\boldsymbol{H}$ such that Eq. (A15) is inexpensive to solve, and the spectral condition number κ' of $\boldsymbol{H}^{-1}\boldsymbol{\Lambda}$ is close to unity. If $\boldsymbol{H}^{-1}$ is a good approximation of $\boldsymbol{\Lambda}^{-1}$ then the second condition will be satisfied; consequently, we look for approximations to $\boldsymbol{\Lambda}$ for which Eq. (A15) is inexpensive to solve.

The operator $\boldsymbol{\Lambda}$ arises from a system of differential equations. For one-dimensional problems a low-order FD approximation to this operator (with grid points coincident with the collocation points) gives rise to a banded system with a small number of bands close to the main diagonal. When this FD operator is used as the preconditioner the system of equations (A15) can be solved efficiently using direct methods.[6]

For instance, in the example considered here [Eq. (A12)] we can set $\boldsymbol{H}$ to be the second-order accurate FD operator corresponding to L. The eigenvalues of the preconditioned operator $\boldsymbol{H}^{-1}\boldsymbol{\Lambda}$ are all in the range $1\leq\lambda_p^{PC}\leq\pi^2/4$: i.e., the spectral condition number is independent of N. In this case the optimal relaxation parameter is

$$\omega'_{\rm opt}\approx\frac{4}{7}, \tag{A16}$$

and each iteration reduces the residual by a factor of approximately 7/3 (independent of N) [13]. The asymptotic cost of finding a solution is thus proportional to the cost of evaluating the residual, $\mathcal{O}(N\ln N)$, which is much more rapid than solution via a direct method or Richardson's iteration without a preconditioner.

For higher dimensional problems the FD preconditioner still leads to a banded system with a small number of nonzero bands; however, some of those bands are found far from the main diagonal and Eq. (A15) can no longer be solved efficiently using direct methods. If N becomes so large that the cost of solving these equations with the FD preconditioner is too great, then the equations for the successive approximations can themselves be solved iteratively, other preconditioners can be explored (cf. [1,2,20]), or the original equations can be solved using another iterative technique, such as multigrid [5]. For the problems considered in this paper N never became so large that a direct solution of Eq. (A15) with the FD preconditioner was problematic.

If Eqs. (A1) are nonlinear, the algebraic equations satisfied by $\boldsymbol{U}$ are similarly nonlinear. Write the nonlinear equations as

$$\boldsymbol{\mathcal{L}}(\boldsymbol{U})=\boldsymbol{F}, \tag{A17}$$

where $\boldsymbol{\mathcal{L}}$ is a nonlinear function of $\boldsymbol{U}$. In order to solve this nonlinear system of equations, we apply Newton's iteration (see Sec. 12.13 and Appendices C and D of Ref. [1]). For Eq. (A5), Newton's iteration is

$$\boldsymbol{\Lambda}_{\boldsymbol{V}^{(i)}}(\boldsymbol{V}^{(i+1)}-\boldsymbol{V}^{(i)})=-\boldsymbol{R}^{(i)}, \tag{A18}$$

[6]For more details on the use of FD operators as preconditioners for spectral problems see [13].

TABLE I. The values of the absolute error Δu_{PSC} of a PSC calculation, as well as the absolute error of a second-order FD calculation Δu_{FD} for several values of N for the example problem [Eq. (A21)]. For $N>16$, the PSC solution is contaminated with roundoff errors.

N	Δu_{PSC}	Δu_{FD}
4	1.7×10^{-1}	2.5×10^{-1}
8	3.2×10^{-4}	5.4×10^{-2}
16	6.9×10^{-10}	1.3×10^{-2}
32	-	3.3×10^{-3}
64	-	8.2×10^{-4}
128	-	2.1×10^{-4}

where $\boldsymbol{\Lambda}_{\boldsymbol{V}^{(i)}}$ is the *linear* operator that arises from linearizing $\boldsymbol{\Lambda}$ about $\boldsymbol{V}^{(i)}$ and $\boldsymbol{R}^{(i)}$ is the *nonlinear* residual given by

$$\boldsymbol{R}^{(i)}=\boldsymbol{\mathcal{L}}(\boldsymbol{U})-\boldsymbol{F}. \tag{A19}$$

Equation (A18) is a linear system to be solved at each step of Newton's iteration. In the same way as before we can introduce a preconditioner, in which case we have the nonlinear Richardson's iteration

$$\boldsymbol{H}(\boldsymbol{V}^{(i+1)}-\boldsymbol{V}^{(i)})=-\omega'\boldsymbol{R}^{(i)}. \tag{A20}$$

Here $\boldsymbol{H}$ is any suitable preconditioning matrix for $\boldsymbol{\Lambda}_{\boldsymbol{V}^{(i)}}$. For the problems solved in Sec. V we used as a preconditioning matrix a second-order accurate FD operator corresponding to the derivative terms of $\mathcal{L}$ *ignoring* the nonlinear terms. (Equivalently we could have used the FD operator corresponding to the linearized operator, but for the problems we examined this was not necessary.)

As a quick demonstration, consider the example problem

$$\frac{d^2u}{dx^2}-e^x[(1-\pi^2)\sin(\pi x)+2\pi\cos(\pi x)]=0, \tag{A21}$$

$$u(-1)=u(1)=0. \tag{A22}$$

We have evaluated approximate solutions to this problem using a second-order accurate FD approximation and a PSC approximation on a Chebyshev basis. For this problem we know the exact solution,

$$u(x)=e^x\sin(\pi x). \tag{A23}$$

Table I lists Δu_{PSC} and Δu_{FD} [cf. Eq. (5.8)] for increasing N (number of grid points for the FD approximation, basis dimension for the PSC approximation). The rapid convergence of PSC is apparent. The second-order FD solution requires 128 points to equal the moderate accuracy of an eighth-order PSC solution. In order to match the high accuracy of the 16th-order PSC solution would require a second-order FD solution with 6.5×10^4 points.

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