Cosmological initial data for numerical relativity

David Garfinkle*
Department of Physics, Oakland University, Rochester, Michigan 48309, USA and Leinweber Center for Theoretical Physics, Randall Laboratory of Physics, University of Michigan, Ann Arbor, Michigan 48109-1120, USA

Lawrence Mead†
School of Mathematics and Natural Sciences, University of Southern Mississippi, Hattiesburg, Mississippi 39406, USA

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We find initial data for numerical relativity simulations of inhomogeneous cosmologies. This involves treating an exceptional case of the general relativity constraint equations. We devise analytic and numerical methods to treat this exceptional case. We apply the analytic method to the standard case of cosmology with a single scalar field. The numerical method is applied to the two-field ekpyrotic cosmology.

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I. INTRODUCTION

Numerical relativity simulations of inhomogeneous cosmologies are performed for a variety of reasons: to explore the inflationary scenario [1–6], or the ekpyrotic scenario [7–10], or the nature of spacetime singularities [11–15], or cosmological structure formation [16–18]. Any simulation must start with initial data, which in general relativity entails solving coupled nonlinear constraint equations [19].

This is very different from the usual treatments of inhomogeneous cosmologies. There the inhomogeneities are typically treated in first order perturbation theory. This allows the perturbations to be separated into modes that decouple and thus can each be treated independently. The initial data can essentially be specified freely.

We would like to have numerical relativity initial data of sufficient generality that they essentially correspond to the sort of initial data used in cosmological perturbation theory. This leads to difficulties, since that sort of data corresponds to an exceptional case in the treatment of the relativity constraint equations. However, we present a method to overcome these difficulties.

In Sec. II we present the constraint equations of general relativity. In Sec. III we specialize to the case relevant to cosmology and show how to overcome the difficulties associated with this exceptional case.

Section IV presents the application of our method to finding numerical relativity initial data that are as close as possible to standard one-field cosmological perturbations. Section V presents a more challenging case associated with the two-field ekpyrotic scenario. Our conclusions are given in Sec. VI.

II. CONSTRAINT EQUATIONS

Initial data for a numerical relativity simulation consist of three-dimensional manifold Σ on which there is a spatial metric γ_{ij} and an extrinsic curvature K_{ij}. Here Σ represents all of the space at the initial time at which the simulation starts. In a phase space picture, γ_{ij} is the configuration variable and K_{ij} is the momentum variable. The data cannot be freely specified, but instead must satisfy two equations called the momentum constraint

$$D^i K_{ij} - D_j K = -\gamma^i{}_j T_{i\mu} n^\mu \tag{1}$$

and the Hamiltonian constraint

$$^{(3)}R + K^2 - K^{ij}K_{ij} = 2T_{\mu\nu}n^\mu n^\nu. \tag{2}$$

Here n^μ is the normal to the initial data surface, D_i is the spatial covariant derivative, and $^{(3)}R$ is the spatial scalar curvature. $T_{\mu\nu}$ is the stress-energy tensor, and we have chosen units where $8\pi G = 1$. Initial data must also be specified for the matter fields that make up $T_{\mu\nu}$.

It is helpful to decompose the extrinsic curvature into its trace K and a trace-free part A_{ij} given by

$$A_{ij} = K_{ij} - \frac{1}{3}K\gamma_{ij}. \tag{3}$$

Then the constraint equations become

*garfinkl@oakland.edu
†Lawrence.Mead@usm.edu

$$D^i A_{ij} - \frac{2}{3} D_j K = -\gamma^i{}_j T_{i\mu} n^\mu, \tag{4}$$

$$^{(3)}R + \frac{2}{3} K^2 - A^{ij} A_{ij} = 2 T_{\mu\nu} n^\mu n^\nu. \tag{5}$$

The constraint equations are usually solved by the York method [19]. This method begins by introducing rescaled quantities $\tilde{\gamma}_{ij}$ and $\tilde{A}_{ij}$ given by

$$\tilde{\gamma}_{ij} = \psi^{-4} \gamma_{ij} \tag{6}$$

and $\tilde{A}_{ij} = \psi^2 A_{ij}$. The quantity $\tilde{A}_{ij}$ is then expressed as

$$\tilde{A}_{ij} = X_{ij} + \tilde{D}_i W_j + \tilde{D}_j W_i - \frac{2}{3} \tilde{\gamma}_{ij} \tilde{\gamma}^{mn} \tilde{D}_m W_n. \tag{7}$$

It seems odd to introduce these new quantities ψ and W_i. However, as we will soon see, they are essentially "correction terms" to be used to convert an initial guess for a solution of the constraint equations into an actual solution.

Using Eqs. (6) and (7) in Eqs. (4) and (5) we obtain

$$\tilde{D}^i \left(\tilde{D}_i W_j + \tilde{D}_j W_i - \frac{2}{3} \tilde{\gamma}_{ij} \tilde{D}^k W_k \right) + \tilde{D}^i X_{ij} - \frac{2}{3} \psi^6 D_j K = -\psi^6 \gamma^i{}_j T_{i\mu} n^\mu, \tag{8}$$

$$\tilde{D}^i \tilde{D}_i \psi - \frac{1}{8} (^{(3)}\tilde{R}) \psi - \frac{1}{12} K^2 \psi^5 + \frac{1}{8} \tilde{A}^{ij} \tilde{A}_{ij} \psi^{-7} = -\frac{1}{4} T_{\mu\nu} n^\mu n^\nu \psi^5. \tag{9}$$

Here spatial indices are raised and lowered with $\tilde{\gamma}_{ij}$. The derivative operator $\tilde{D}_i$ and scalar $^{(3)}\tilde{R}$ are, respectively, the covariant derivative and scalar curvature associated with $\tilde{\gamma}_{ij}$.

For our purposes, it is helpful to think of the quantities used in the York method as follows: K is to be freely specified. $\tilde{\gamma}_{ij}$ and X_{ij} are our initial guesses for γ_{ij} and A_{ij}. That is, if we happened to have (γ_{ij}, A_{ij}) satisfying Eqs. (4) and (5) then the choice $\psi = 1$ and $W_i = 0$ would solve Eqs. (8) and (9). If our initial guess does not solve the constraint equations, then W_i and ψ are correction terms that turn our initial guess into a solution. That is, by solving Eqs. (8) and (9) for W_i and ψ we obtain a solution of Eqs. (4) and (5). So our task of solving the constraint equations has reduced to the task of solving Eqs. (8) and (9) for W_i and ψ.

As it stands, Eqs. (8) and (9) are coupled, nonlinear differential equations. However, the standard procedure decouples them as follows: first define the quantity $\tilde{J}_j$ by

$$\tilde{J}_j = \psi^6 \gamma^i{}_j T_{i\mu} n^\mu. \tag{10}$$

For each choice of matter fields, we must choose a way of specifying initial data so that $\tilde{J}_j$ does not depend on ψ. In Sec. IV we will give an explicit example of how to perform this sort of specification.

Second, choose K to be constant, so that $\tilde{D}_i K = 0$. This choice of K to be constant sounds like a loss of generality in the choice of initial data, but it turns out that it is not, for the following reason: the result of evolving the initial data in a numerical relativity simulation will be a spacetime. But spacetime can be divided up into space and time in many different ways. One such way is to have the surfaces of constant time be surfaces of constant K. So in choosing constant K for our initial data surface, we are simply making use of the coordinate invariance of general relativity. Or to put it another way: general relativity has gauge freedom, and we are choosing a convenient gauge.

With these choices, Eq. (8) becomes

$$\tilde{D}^i \left(\tilde{D}_i W_j + \tilde{D}_j W_i - \frac{2}{3} \tilde{\gamma}_{ij} \tilde{D}^k W_k \right) = -\tilde{D}^i X_{ij} - \tilde{J}_j. \tag{11}$$

This is a linear equation for W_i that does not depend on ψ. So the idea is to first solve Eq. (11) for W_i and then plug the result into Eq. (9) which is to be solved for ψ. Equation (9) is a somewhat complicated looking nonlinear equation. But it is straightforward to solve it using standard numerical methods for nonlinear elliptic equations. Therefore, for the rest of the paper we will only concentrate on how to solve Eq. (11).

Equation (11) is of the form operator acting on W_i equals source, so the first thing we want to know is, does the operator have a kernel? That is, is there a vector V_i for which

$$\tilde{D}^i \left(\tilde{D}_i V_j + \tilde{D}_j V_i - \frac{2}{3} \tilde{\gamma}_{ij} \tilde{D}^k V_k \right) = 0? \tag{12}$$

If there is no kernel, then the operator can be inverted and therefore there exists a unique solution of Eq. (11). Multiplying Eq. (12) by V^j and integrating over Σ using integration by parts we have

$$\int_\Sigma (\tilde{D}^i V^j) \left(\tilde{D}_i V_j + \tilde{D}_j V_i - \frac{2}{3} \tilde{\gamma}_{ij} \tilde{D}^k V_k \right) = 0. \tag{13}$$

But this can be the case only if at each point we have

$$\tilde{D}_i V_j + \tilde{D}_j V_i - \frac{2}{3} \tilde{\gamma}_{ij} \tilde{D}^k V_k = 0. \tag{14}$$

Equation (14) is the conformal Killing equation. Its solutions are conformal Killing vector fields. But spaces with conformal Killing vectors are rare. Thus the conclusion for Eq. (11) is that there is a general case (no conformal Killing vectors) in which there exists a unique solution, and then there is an exceptional case in which there is a conformal Killing vector.

III. COSMOLOGICAL CASE

Unfortunately, the exceptional case, although in some sense rare, is also the one of most relevance for cosmology. Cosmological scalar perturbations have a conformally flat spatial metric. A conformally flat metric has conformal Killing vector fields. We are therefore led to investigate the exceptional case, and in fact to further specialize to the case where the conformally related metric $\tilde{\gamma}_{ij}$ is the flat metric δ_{ij} (i.e., the Kronecker delta). Equation (11) then becomes

$$\partial^i\left(\partial_i W_j + \partial_j W_i - \frac{2}{3}\delta_{ij}\partial^k W_k\right) = -\partial^i X_{ij} - \tilde{J}_j. \quad (15)$$

Here ∂_i is the usual Cartesian coordinate derivative operator.

For linear equations where there is a kernel, we have the Fredholm alternative: any vector is expressed as the sum of two pieces, one in the kernel and one in the space orthogonal to the kernel (called the adjoint). If the source is not in the adjoint, then the linear equation has no solutions. If the source is in the adjoint, then the linear equation has multiple solutions, where any two solutions differ by something in the kernel.

Our task in solving Eq. (15) is therefore to first put conditions on the matter field initial data that ensure that the right-hand side of the equation is in the adjoint. We must then find what is essentially the inverse of the operator on the adjoint space, in order to find a solution of Eq. (15). There will be multiple solutions. However, using the fact that any two solutions differ by something in the kernel, an examination of Eq. (7) shows that the two solutions give rise to the same $\tilde{A}_{ij}$, so in fact we can pick any solution, and it does not matter which one we pick.

A single mode in cosmological perturbation theory has spatial dependence only in the direction of propagation. So we now further specialize to the case where there is dependence on only the x coordinate. We want initial data for a simulation with periodic boundary conditions, so we choose x to be a periodic coordinate with period 2π. We choose $W_y = W_z = 0$. [That is, we consider only choices of X_{ij} for which the solution of Eq. (15) gives $W_y = W_z = 0$.] Equation (15) then becomes

$$\frac{4}{3}\frac{d^2 W_x}{dx^2} = -\frac{dX_{xx}}{dx} - \tilde{J}_x. \quad (16)$$

In some cases, the right-hand side of Eq. (16) is sufficiently simple that the equation can be solved in closed form. However, other cases require a numerical method. For similar equations, but ones without a kernel, the standard numerical method is to write the finite difference approximation of the equation as a matrix equation and then to perform an LU decomposition of the matrix [20]. However, Eq. (16) does have a kernel, since a constant W_x gives zero for the left-hand side of the equation. And indeed, application of the formula of [20] to this case results in division by zero. Instead, we use a different type of LU decomposition method, described in Appendix A, for the numerical solution of Eq. (16).

Whether solved analytically or numerically, a solution of Eq. (16) for W_x gives rise to an expression for $\tilde{A}_{ij}$, which can in turn be used to solve Eq. (9) for ψ. The expression is $\tilde{A}_{ij} = X_{ij}$ for $i \neq j$ and

$$\tilde{A}_{xx} = X_{xx} + \frac{4}{3}\frac{dW_x}{dx}, \quad (17)$$

$$\tilde{A}_{yy} = X_{yy} - \frac{2}{3}\frac{dW_x}{dx}, \quad (18)$$

$$\tilde{A}_{zz} = X_{zz} - \frac{2}{3}\frac{dW_x}{dx}. \quad (19)$$

IV. STANDARD ONE-FIELD CASE

We now treat the case of cosmology with scalar field matter. Here we will find that Eq. (16) can be solved in closed form. We want to find initial data that are as close as possible to a single mode of a cosmological scalar perturbation. The stress energy of the scalar field ϕ with potential $V(\phi)$ is

$$T_{\mu\nu} = \nabla_\mu\phi\nabla_\nu\phi - g_{\mu\nu}\left(\frac{1}{2}\nabla^\alpha\phi\nabla_\alpha\phi + V\right). \quad (20)$$

Now using Eq. (20) in Eq. (10) we find

$$\tilde{J}_j = \psi^6 P\partial_j\phi, \quad (21)$$

where the quantity P is defined by $P = n^\mu\nabla_\mu\phi$. To make $\tilde{J}_j$ independent of ψ we define the quantity Q by

$$Q = \psi^6 P, \quad (22)$$

which leads to

$$\tilde{J}_j = Q\partial_j\phi. \quad (23)$$

So we specify Q, and it is only at the end, when we have numerically solved for ψ, that we know the stress energy.

We will find the initial values for Q and ϕ of a cosmological scalar perturbation, and use those in Eqs. (16) and (23) to find the general relativity initial data.

The background Friedmann-Lemaitre-Robertson-Walker (FLRW) spacetime has the line element

$$ds^2 = -dt^2 + a^2(t)(dx^2 + dy^2 + dz^2). \quad (24)$$

We will denote quantities in the background with a subscript zero and use an overdot for the derivative with respect to t. The Hubble parameter H is given by $H = \dot{a}/a$. Then we have

$$K_0 = -3H, \tag{25}$$

$$Q_0 = a^3\dot{\phi}_0. \tag{26}$$

A single mode of the scalar field is usually written as a function of time multiplied by e^{iqx}, with the notion that since the equations are linear, we can do all our computations with the complex mode and at the end of the day we will take the real part. However, $\tilde{J}_j$ is quadratic in the scalar field, not linear, so we will write our modes as real quantities from the start. Since we have chosen x to be a periodic variable going from 0 to 2π, therefore q will be an integer. The quantities ϕ and Q take the form

$$\phi = \phi_0 + c_1\cos(qx) + c_2\sin(qx), \tag{27}$$

$$Q = Q_0 + c_3\cos(qx) + c_4\sin(qx), \tag{28}$$

where c_1, c_2, c_3, and c_4 are constants.

Cosmological scalar perturbations have $X_{ij} = 0$, so Eq. (16) becomes

$$\frac{4}{3}\frac{d^2W_x}{dx^2} = -\tilde{J}_x. \tag{29}$$

Using Eqs. (27) and (28) in Eq.. (23) we obtain

$$\begin{aligned} -\tilde{J}_x &= q(Q_0 + c_3\cos(qx) + c_4\sin(qx)) \\ &\quad\times(c_1\sin(qx) - c_2\cos(qx)) \end{aligned} \tag{30}$$

$$\begin{aligned} &= Q_0 q[c_1\sin(qx) - c_2\cos(qx)] \\ &\quad + \frac{1}{2}q[(c_1c_4 - c_2c_3) - (c_1c_4 + c_2c_3)\cos(2qx) \\ &\quad + (c_1c_3 - c_2c_4)\sin(2qx)]. \end{aligned} \tag{31}$$

The requirement that the source be in the adjoint means that the constant term on the right-hand side of Eq. (31) must vanish. That is, we must require

$$c_1c_4 = c_2c_3. \tag{32}$$

This sort of constraint on the freedom to specify a cosmological perturbation is known as an integral constraint [21].

Using Eq. (31) in Eq. (29) and integrating, we obtain

$$\begin{aligned} \frac{4}{3}\frac{dW_x}{dx} &= -Q_0[c_1\cos(qx) + c_2\sin(qx)] \\ &\quad - \frac{1}{4}[(c_1c_4 + c_2c_3)\sin(2qx) \\ &\quad + (c_1c_3 - c_2c_4)\cos(2qx)]. \end{aligned} \tag{33}$$

This is our solution of the momentum constraint equation.

We will now express the parameters (c_1, c_2, c_3, c_4) in terms of the standard cosmological perturbation theory [22,23] in Newtonian gauge.

The line element in Newtonian gauge takes the form

$$ds^2 = -(1+2\Psi)dt^2 + a^2(1-2\Psi)\delta_{ij}dx^i dx^j, \tag{34}$$

where Ψ is the cosmological Newtonian potential.

The scalar field in Newtonian gauge takes the form

$$\phi_N = \phi_0 + \alpha(t)\cos(qx) + \beta(t)\sin(qx). \tag{35}$$

From Eq. (34) we find that Q and K in Newtonian gauge are

$$Q_N = a^3\dot{\phi}_0(1-4\Psi) + a^3(\dot{\alpha}\cos(qx) + \dot{\beta}\sin(qx)), \tag{36}$$

$$K_N = -3H + 3(\dot{\Psi} + H\Psi). \tag{37}$$

It is clear from Eq. (37) that K_N has dependence on the spatial coordinates, and therefore that Newtonian gauge is not constant mean curvature (CMC) gauge. However, we can transform to CMC gauge through the use of a gauge transformation. In general relativistic perturbation theory, for every vector field ξ^μ there is a gauge transformation that consists of adding to each quantity Lie derivative with respect to ξ^μ of the background quantity. We will choose our vector field to have only a time component. The gauge transformed K is then

$$\begin{aligned} K &= K_N + \mathcal{L}_\xi K_0 \\ &= -3H + 3(\dot{\Psi} + H\Psi) + \xi^t\partial_t(-3H) \\ &= 3(-H + \dot{\Psi} + H\Psi - \xi^t\dot{H}). \end{aligned} \tag{38}$$

Thus to make K spatially constant, we choose ξ^t to be

$$\xi^t = \frac{\dot{\Psi} + H\Psi}{\dot{H}}. \tag{39}$$

However, a standard result of cosmological perturbation theory in Newtonian gauge is [23]

$$\dot{\Psi} + H\Psi = \frac{1}{2}\dot{\phi}_0(\phi_N - \phi_0) \tag{40}$$

so we find

$$\xi^t = \frac{\dot{\phi}_0}{2\dot{H}}(\phi_N - \phi_0). \tag{41}$$

Applying the gauge transformation, we find that the scalar field in CMC gauge is

$$\begin{aligned}\phi &= \phi_N + \mathcal{L}_\xi \phi_0 = \phi_N + \xi^t \dot{\phi}_0 \\ &= \phi_0 + \left(1 + \frac{\dot{\phi}_0^2}{2\dot{H}}\right)(\phi_N - \phi_0) \\ &= \phi_0 + \left(1 + \frac{\dot{\phi}_0^2}{2\dot{H}}\right)(\alpha \cos(qx) + \beta \sin(qx)). \end{aligned} \tag{42}$$

Comparing Eqs. (27) and (42) we see that two of the parameters of our momentum constraint solution are given by

$$c_1 = \left(1 + \frac{\dot{\phi}_0^2}{2\dot{H}}\right)\alpha, \qquad c_2 = \left(1 + \frac{\dot{\phi}_0^2}{2\dot{H}}\right)\beta, \tag{43}$$

where all quantities are evaluated at the time t_0 of our initial data.

We now find the quantity Q in CMC gauge. We have

$$\begin{aligned} Q &= Q_N + \mathcal{L}_\xi Q_0 = Q_N - Q_0 \frac{V'(\phi_0)}{\dot{\phi}_0} \xi^t \\ &= Q_N - Q_0 \frac{V'(\phi_0)}{2\dot{H}} (\phi - \phi_N), \end{aligned} \tag{44}$$

where we have used the equation of motion for the background scalar field.

To evaluate the term proportional to Ψ in the expression of Eq. (28) for Q_N, we use the following result of cosmological perturbation theory in Newtonian gauge [23]:

$$(\dot{H} + q^2/a^2)\Psi = \frac{1}{2}\ddot{\phi}_0(\phi_N - \phi_0) - \frac{1}{2}\dot{\phi}_0(\dot{\phi}_N - \dot{\phi}_0). \tag{45}$$

Combining Eqs. (28), (44), and (45) we obtain

$$\begin{aligned} Q = Q_0 &+ a^3 \left(1 + \frac{2\dot{\phi}_0^2}{\dot{H} + q^2/a^2}\right)(\dot{\alpha}\cos(qx) + \dot{\beta}\sin(qx)) \\ &- a^3 \dot{\phi}_0 \left(\frac{V'(\phi_0)}{2\dot{H}} + \frac{2\ddot{\phi}_0}{\dot{H} + q^2/a^2}\right)(\alpha \cos(qx) + \beta \sin(qx)). \end{aligned} \tag{46}$$

Comparing Eqs. (28) and (46) we find that the remaining two parameters of our momentum constraint solution are given by

$$\begin{aligned} c_3 &= a^3 \left(1 + \frac{2\dot{\phi}_0^2}{\dot{H} + q^2/a^2}\right)\dot{\alpha} - a^3 \dot{\phi}_0 \left(\frac{V'(\phi_0)}{2\dot{H}} + \frac{2\ddot{\phi}_0}{\dot{H} + q^2/a^2}\right)\alpha, \\ c_4 &= a^3 \left(1 + \frac{2\dot{\phi}_0^2}{\dot{H} + q^2/a^2}\right)\dot{\beta} - a^3 \dot{\phi}_0 \left(\frac{V'(\phi_0)}{2\dot{H}} + \frac{2\ddot{\phi}_0}{\dot{H} + q^2/a^2}\right)\beta, \end{aligned} \tag{47}$$

where all quantities are evaluated at the time t_0 of our initial data.

Using Eqs. (43) and (47), we see that the constraint on the parameters $c_1 c_4 = c_2 c_3$ becomes

$$\alpha\dot{\beta} = \beta\dot{\alpha}. \tag{48}$$

V. EKPYROTIC TWO-FIELD CASE

We now treat the case of the ekpyrotic two-field model [24]. In this model there is a scalar field ϕ with a potential $V(\phi)$ and thus the same stress energy as in Eq. (20). However, there is also a second scalar field χ whose kinetic term is coupled to the first scalar field through a function $\kappa(\phi)$. In the ekpyrotic scenario, ϕ causes the smoothing during a contracting phase prior to the bounce into the big bang, while ϕ and χ together ensure the appropriate spectrum of perturbations. The combined stress energy of the two fields is

$$\begin{aligned} T_{\mu\nu} = \nabla_\mu \phi \nabla_\nu \phi - g_{\mu\nu}\left(\frac{1}{2}\nabla^\alpha \phi \nabla_\alpha \phi + V\right) \\ + \kappa(\phi)\left[\nabla_\mu \chi \nabla_\nu \chi - \frac{1}{2} g_{\mu\nu} \nabla^\alpha \chi \nabla_\alpha \chi\right]. \end{aligned} \tag{49}$$

As before, we define P and Q by $P = n^\mu \nabla_\mu \phi$ and $Q = \psi^6 P$. However, we also define P_χ and Q_χ by $P_\chi = n^\mu \nabla_\mu \chi$ and $Q_\chi = \psi^6 P_\chi$. Since we are concerned with scalar modes, we will choose $X_{ij} = 0$. Then the momentum constraint once again takes the form

$$\frac{4}{3}\frac{d^2 W_x}{dx^2} = -\tilde{J}_x. \tag{50}$$

But now with $\tilde{J}_x$ taking the form

$$\tilde{J}_x = Q\partial_x \phi + \kappa(\phi) Q_\chi \partial_x \chi. \tag{51}$$

In this case, we are not so much concerned with matching a particular perturbative mode, but rather with coming up with a class of initial data, not necessarily small, of sufficient generality to allow a thorough numerical exploration of the two-field ekpyrotic scenario. The condition needed for a solution of Eq. (50), namely that $\tilde{J}_x$ be in the adjoint, becomes

$$\int_0^{2\pi} dx\, \tilde{J}_x = 0. \tag{52}$$

One simple way to satisfy this condition is to make ϕ, χ, Q, and Q_χ functions of $\cos x$. In this way, both $Q\partial_x \phi$ and $\kappa(\phi) Q_\chi \partial_x \chi$ become odd functions of x, whose integral over one period therefore vanishes. We will take the usual choice for $\kappa(\phi)$ of

$$\kappa(\phi) = e^{-c\phi}, \tag{53}$$

where c is a constant. For nonperturbative initial data, we cannot solve Eq. (50) in closed form. Therefore instead we use the numerical method presented in Appendix A. If we were doing a perturbative treatment, we would replace $e^{-c\phi}$ with $1 - c\phi$ and solve Eq. (50) using the analytic methods of the previous section. Figures 1 and 2 show the results of such a numerical solution. Here we have used ϕ, χ, Q, and Q_χ of the form $\phi = c_0 \cos(qx)$, $Q = c_1 \cos(qx)$, $\chi = d_0 \cos(qx)$, $Q_\chi = d_1 \cos(qx)$. We plot the results of the numerical treatment in a solid line and the results of the corresponding perturbative-analytic treatment in a dashed line. In Fig. 1 we pick parameters $c = 5$, $q = 1$, $c_0 = 0.1$, $c_1 = 0.2$, $d_0 = 0.2$, $d_1 = 0.3$, which correspond to weak initial data. Note that in this case the perturbative result is quite close to the numerical result. In contrast, in Fig. 2 we pick parameters $c = 5$, $q = 1$, $c_0 = 1.0$, $c_1 = 1.4$, $d_0 = 2.0$, $d_1 = 1.6$ corresponding to much stronger initial data. Here the perturbative result is not at all a good approximation for the full numerical treatment, and so the numerical method is definitely needed.

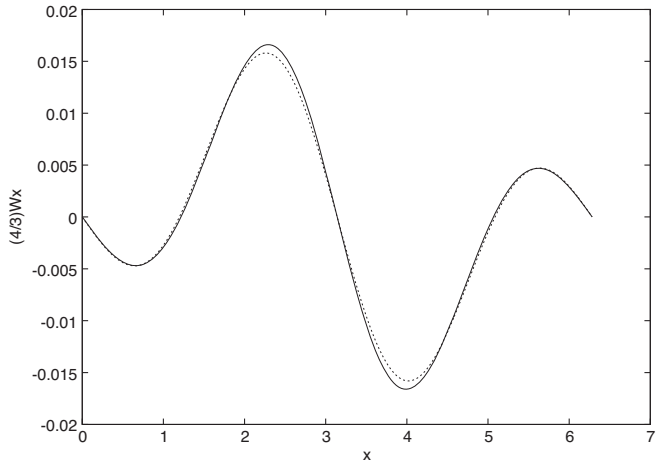

FIG. 1. $(4/3)W_x$ vs x for the numerical method (solid line) and perturbative method (dashed line) for weak initial data.

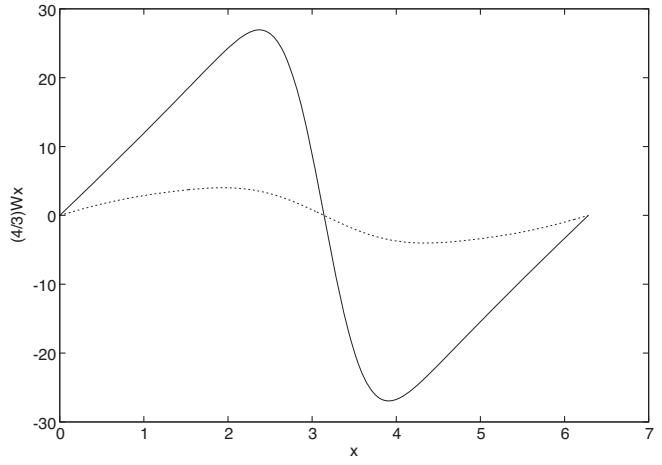

FIG. 2. $(4/3)W_x$ vs x for the numerical method (solid line) and perturbative method (dashed line) for strong initial data.

VI. CONCLUSION

We have provided methods to generate more extensive sets of initial data for numerical relativity simulations of inhomogeneous cosmologies. The sort of data needed for inhomogeneous cosmologies constitute an exceptional case within the York method for finding general relativity initial data. Because it is exceptional, this case cannot be treated using the standard numerical methods. Nonetheless, we have found some situations where the problem can be solved in closed form. And for the situations that cannot be treated in closed form, we have found a numerical method, a subtle modification of the standard LU decomposition method, that works.

Typically the goal of numerical relativity simulations of inhomogeneous cosmologies is to make assertions about what outcomes result from "generic" initial conditions. But this means that the wider the class of initial data used for the simulations, the more confidently one can assert that the simulations give the generic outcome. It would be interesting to repeat some of the simulations of inhomogeneous cosmologies (e.g., some of the ones given in the references of this paper) with our more general initial data to see if the conclusions about outcomes remain the same.

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APPENDIX: NUMERICAL METHOD

We need to numerically solve an equation of the form

$$\frac{d^2 f}{dx^2} = g \tag{A1}$$

on a grid with periodic boundary conditions. We pick N grid points with spacing Δ and denote with a subscript i the value of the function at grid point i. Using centered differences, Eq. (A1) becomes

$$\frac{f_{i+1} + f_{i-1} - 2f_i}{\Delta^2} = g_i. \tag{A2}$$

This equation can be used at all grid points except grid points 1 and N. To evaluate Eq. (A1) at these points, we add two ghost zones, grid points 0 and $N + 1$ that implement the periodic boundary conditions: $f_0 = f_N$ and $f_{N+1} = f_1$. We then find

$$\Delta^2 g_1 = f_2 + f_0 - 2f_1 = f_2 + f_N - 2f_1, \tag{A3}$$

$$\Delta^2 g_N = f_{N+1} + f_{N-1} - 2f_N = f_1 + f_{N-1} - 2f_N. \tag{A4}$$

Using the notation $|f\rangle$ for the column vector of f_i and similarly for $|g\rangle$ we find that Eq. (A2) with periodic boundary conditions applied can be written as the matrix equation $A|f\rangle = \Delta^2|g\rangle$ where for definiteness we display the matrix A for the case $N = 4$:

$$A = \begin{pmatrix} -2 & 1 & 0 & 1 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 1 & 0 & 1 & -2 \end{pmatrix}. \tag{A5}$$

If A were invertible, we could solve for $|f\rangle$ by multiplying both sides of the equation $A|f\rangle = \Delta^2|g\rangle$ by A^{-1}. However, it is easy to see that A is not invertible, since it annihilates the vector $|f\rangle$ where all the f_i are equal to the same constant. This is just the finite difference version of the statement that the operator d^2/dx^2 annihilates the function f that is a constant.

For an invertible matrix, there is a standard decomposition of the matrix into lower and upper triangular matrices (called LU decomposition) that allows a convenient algorithm [20] for solving the system of linear equations associated with the matrix. The matrix A is not invertible, but, nonetheless, we have an analog of the LU decomposition, which we display for the $N = 4$ case: $A = LU$ where

$$L = \begin{pmatrix} -1 & 0 & 0 & 1 \\ 1 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 1 & -1 \end{pmatrix}, \tag{A6}$$

$$U = \begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 1 & -1 \\ -1 & 0 & 0 & 1 \end{pmatrix}. \tag{A7}$$

Note that despite their names, the matrix L is not lower triangular because of the entry in the upper right-hand corner, and the matrix U is not upper triangular because of the entry in the lower left-hand corner.

As with standard LU decomposition, the idea is that to solve the equation $LU|x\rangle = |r\rangle$ for $|x\rangle$, we first solve $L|y\rangle = |r\rangle$ for $|y\rangle$ and then solve $U|x\rangle = |y\rangle$ for $|x\rangle$. We will work out this problem explicitly for the $N = 4$ case illustrated in Eqs. (A5)–(A7). Then we will describe the corresponding algorithm for general N. The equation $L|y\rangle = |r\rangle$ becomes the following set of linear equations:

$$-y_1 + y_4 = r_1, \tag{A8}$$

$$y_1 - y_2 = r_2, \tag{A9}$$

$$y_2 - y_3 = r_3, \tag{A10}$$

$$y_3 - y_4 = r_4. \tag{A11}$$

Adding Eqs. (A8)–(A11) we obtain $r_1 + r_2 + r_3 + r_4 = 0$. In other words $|r\rangle$ must be in the adjoint, which is what the Fredholm alternative tells us needs to be true anyway if there is to be a solution to the original problem $A|x\rangle = |r\rangle$.

Notice that the left-hand sides of Eqs. (A8)–(A11) are each differences of two y_i. This means that if we have a solution of these equations, then we can obtain another solution simply by adding the same constant to each y_i. We will exploit this freedom to choose $y_4 = 0$. Note that Eq. (A8) then yields $y_1 = -r_1$. But knowing y_1 now allows us to solve Eq. (A9) for y_2, which in turn allows us to solve Eq. (A10) for y_3. This solution for the y_i is then

$$|y\rangle = \begin{pmatrix} -r_1 \\ -(r_1 + r_2) \\ -(r_1 + r_2 + r_3) \\ 0 \end{pmatrix}. \tag{A12}$$

Note that the average value of the y_i is then $\bar{y} = (-1/4)(3r_1 + 2r_2 + r_3)$. We will produce a new solution by subtracting this average from each y_i and thus have a solution where the sum of the y_i vanishes. (As we will soon see, we will need this solution in order to solve the equation $U|x\rangle = |y\rangle$.) The new solution is

$$|y\rangle = \frac{1}{4}\begin{pmatrix} -r_1 + 2r_2 + r_3 \\ -r_1 - 2r_2 + r_3 \\ -r_1 - 2r_2 - 3r_3 \\ 3r_1 + 2r_2 + r_3 \end{pmatrix}. \tag{A13}$$

The equation $U|x\rangle = |y\rangle$ becomes the following set of linear equations:

$$x_1 - x_2 = y_1, \tag{A14}$$

$$x_2 - x_3 = y_2, \tag{A15}$$

$$x_3 - x_4 = y_3, \tag{A16}$$

$$-x_1 + x_4 = y_4. \tag{A17}$$

Adding Eqs. (A14)–(A17) we obtain $y_1+y_2+y_3+y_4=0$. In other words, we did need to impose the condition that $|y\rangle$ is in the adjoint on the previous solution.

Since the left-hand sides of Eqs. (A14)–(A17) are each differences of two x_i, we can obtain from any solution another solution simply by adding the same constant to each x_i. We will exploit this freedom to choose $x_1 = 0$. Note that Eq. (A17) then yields $x_4 = y_4$. But knowing x_4 now allows us to solve Eq. (A16) for x_3, which in turn allows us to solve Eq. (A15) for x_2. This solution for the x_i is then

$$|x\rangle = \begin{pmatrix} 0 \\ y_2 + y_3 + y_4 \\ y_3 + y_4 \\ y_4 \end{pmatrix}. \tag{A18}$$

Note that the average value of the x_i is then $\bar{x} = (1/4)(y_2 + 2y_3 + 3y_4)$. Though not strictly necessary, we will proceed in analogy to our previous method for finding $|y\rangle$ and produce a new solution for $|x\rangle$ by subtracting this average from each x_i and thus have a solution where the sum of the x_i vanishes. The new solution is

$$|x\rangle = \frac{1}{4}\begin{pmatrix} -y_2 - 2y_3 - 3y_4 \\ 3y_2 + 2y_3 + y_4 \\ -y_2 + 2y_3 + y_4 \\ -y_2 - 2y_3 + y_4 \end{pmatrix}. \tag{A19}$$

Finally, using Eq. (A13) in Eq. (A19) we obtain the solution to the original problem $LU|x\rangle = |r\rangle$:

$$|x\rangle = \frac{1}{8}\begin{pmatrix} -3r_1 + r_3 \\ -r_1 - 4r_2 - r_3 \\ r_1 - 3r_3 \\ 3r_1 + 4r_2 + 3r_3 \end{pmatrix}. \tag{A20}$$

This solution can also be expressed in a slightly more natural looking way using $r_1 + r_2 + r_3 + r_4 = 0$ as

$$|x\rangle = \frac{1}{8}\begin{pmatrix} r_3 - 3r_1 \\ r_4 - 3r_2 \\ r_1 - 3r_3 \\ r_2 - 3r_4 \end{pmatrix}. \tag{A21}$$

We now describe the general form of the algorithm to obtain this solution (i.e., for general N, not restricted to $N = 4$). The kernel of A consists of all $|f\rangle$ where the f_i all have the same values. The adjoint of A consists of all $|f\rangle$ where $\sum_{i=1}^{N} f_i = 0$. This kernel of A is also the kernel of L and U, and the adjoint of A is also the adjoint of L and U. The vector $|r\rangle$ must be in the adjoint, or there is no solution of $L|y\rangle = |r\rangle$. But if $|r\rangle$ is in the adjoint, then there are multiple solutions for $|y\rangle$ each differing by something in the kernel. We make use of this freedom to choose $y_N = 0$. It then follows that $y_1 = -r_1$ and that $y_{i+1} = y_i - r_{i+1}$, which we iteratively solve in succession for $y_2, y_3, \ldots, y_{N-1}$. This $|y\rangle$ is generally not in the adjoint, which would make it impossible to solve $U|x\rangle = |y\rangle$. However, we turn it into a solution in the adjoint by subtracting the appropriate vector in the kernel. That is, we find the average $\bar{y}$ of the y_i and then subtract $\bar{y}$ from each y_i to make our new vector $|y\rangle$. Now we use the same sort of procedure to solve $U|x\rangle = |y\rangle$. We use the freedom to add something in the kernel to choose $x_1 = 0$. We then have $x_N = y_N$, as well as $x_{i-1} = x_i + y_{i-1}$ which we solve iteratively for $x_{N-1}, x_{N-2}, \ldots, x_2$. This $|x\rangle$ is a solution of the equation $A|x\rangle = |r\rangle$ but we go ahead and produce a solution in the adjoint by subtracting $\bar{x}$ from each x_i.

This algorithm may sound a bit complicated, but it is straightforward to program and the resulting code is about the same length as the general description given above of the algorithm.

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