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Multigrid elliptic equation solver with adaptive mesh refinement

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Abstract

In this paper, we describe in detail the computational algorithm used by our parallel multigrid elliptic equation solver with adaptive mesh refinement. Our code uses truncation error estimates to adaptively refine the grid as part of the solution process. The presentation includes a discussion of the orders of accuracy that we use for prolongation and restriction operators to ensure second order accurate results and to minimize computational work. Code tests are presented that confirm the overall second order accuracy and demonstrate the savings in computational resources provided by adaptive mesh refinement.

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1. Introduction

Elliptic equations appear throughout engineering, science, and mathematics. Our primary interest is in elliptic problems that arise in the context of numerical relativity. Currently, the field of numerical relativity is being driven by rapid progress on the experimental front. There are several ground-based gravitational wave detectors in operation today, and their sensitivities are quickly approaching a level at which interesting science can be done. There are also plans for a space-based gravitational wave detector, LISA, to be launched around 2012. The scientific payoff of these instruments will depend largely on our ability to theoretically predict and explain the observed signals. For both ground-based and space-based gravitational wave detectors, the most common and strongest signals are expected to come from colliding black holes. Thus, much of the numerical relativity community has directed its efforts toward modeling binary black hole systems.

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When black holes spiral together and collide, they generate gravitational waves. The black hole "source" region has a length scale of GM/c^2 , where G is Newton's constant, M is the total mass of the two black holes, and c is the speed of light. The gravitational waves produced by the source have a length scale up to $\sim 100GM/c^2$. Herein lies one of the challenges of modeling binary black hole systems with finite difference methods. The source region requires grid zones of size $\leq 0.01GM/c^2$ to accurately capture the details of the black holes' interaction, while the extent of the grid needs to be several hundred GM/c^2 to accurately capture the details of the gravitational wave signal. Many research groups in numerical relativity are starting to use adaptive mesh refinement (AMR) techniques to deal with this discrepancy in length scales [1–11]. With AMR the grid resolution is allowed to vary across the computational domain so that computational resources can be concentrated where they are most needed. For the binary black hole problem, we need a high resolution region to cover the small-scale detail of the source, but the gravitational waves far from the source can be modeled with sufficient accuracy using a much lower resolution grid.

Elliptic equations occur in several contexts in numerical relativity. Einstein's theory of gravity is a system of partial differential equations consisting of four constraint equations and a set of evolution equations (see for example [12]). The constraint equations restrict the data at each time step so in particular the initial data cannot be chosen freely. With suitable assumptions about the nature of the initial data, the constraint equations can be written as an elliptic system [13].

Having solved the constraints for the initial data, those data are evolved forward in time by the evolution equations. At an analytical level, the evolution equations guarantee that the constraint equations will continue to be satisfied. However, in numerical modeling, numerical errors will introduce violations of the constraints. These violations can be disastrous because the evolution equations admit unphysical, constraint violating solutions that grow exponentially [14–17]. One possible strategy for preventing this disaster is to impose the constraints during the evolution, which means solving the elliptic constraint equations after each time step [18–20].

Elliptic equations also arise in numerical relativity when one is faced with choosing a coordinate system. In Einstein's theory the coordinate system must be chosen dynamically as the gravitational field evolves forward in time. The choice of coordinate system can have a dramatic effect on the performance of a numerical relativity code. Researchers have developed many different strategies for choosing a coordinate system. Some of these strategies require the solution of elliptic, parabolic or hyperbolic equations, and some involve algebraic conditions. Some researchers feel that the elliptic conditions might be best, but the cost of solving elliptic equations at each time step has made the other choices more practical and more popular.

In the numerical relativity community we need the capability of solving elliptic equations quickly on adaptive, non-uniform grids. No doubt this same need exists in other areas of science and applied mathematics.

Multigrid methods originated in the 1960s with the work of Fedorenko and Bakhvalov [21–23]. They were further developed in the 1970s by Brandt [24,25], and are now the preferred methods for solving elliptic partial differential equations. The advantage of multigrid is its speed – multigrid algorithms only require order N^3 operations to solve an elliptic equation, where N^3 is the number of grid points. In this paper, we describe our code, AMRMG, which solves nonlinear elliptic equations using multigrid methods with adaptive mesh refinement. The idea of combining multigrid with AMR is not new [24–27], although there are a number of features of our code that distinguish it from the discussions we have seen. In particular, AMRMG uses cell-centered data, as opposed to node centered data. AMRMG uses the full approximation storage (FAS) algorithm, and therefore is not restricted to linear elliptic equations. AMRMG uses the Paramesh package to implement parallelization and to organize the multigrid structure [28,29]. In [30], we used AMRMG to solve numerically for distorted black hole initial data.

AMRMG is currently set up to solve second order equations that are semi-linear (the second order derivative terms are linear in the unknown field). The FAS scheme is applicable for fully nonlinear equations as well, and in principle AMRMG can be modified to solve any nonlinear equation. The equations of current interest for us are semi-linear, therefore we have not tested AMRMG on any fully nonlinear systems.

In this paper, we describe the algorithm behind AMRMG in detail. In Section 2, we present the overall conceptual framework behind our code, and discuss some of the choices made in its development. Section 3 is devoted to a discussion of guard cell filling, which determines the coupling between fine and coarse grid regions. In Section 4, we review the FAS algorithm and in Section 5, we discuss in detail the restriction and prolongation operators used by AMRMG. In Section 6, we describe the calculation of the relative truncation error and how it is used to control the grid structure. Section 7 contains the results of a number of code tests involving the calculation of initial data for numerical relativity.

2. Multigrid with AMR

The simplest technique for solving an elliptic problem is relaxation. The equation (or system of equations) is written in discrete form as $f_i(\phi) = g_i(\phi)$, where *i* labels the grid points and ϕ_i denotes the numerical solution. A "relaxation sweep" consists of refining the approximate solution ϕ_i^{old} by solving the system $f_i(\phi^{\text{new}}) = g_i(\phi^{\text{old}})$ for ϕ_i^{new} . [In the simplest case *f* is the identity and relaxation is written as $\phi_i^{\text{new}} = g_i(\phi^{\text{old}})$.] The success of the relaxation method depends on how the finite difference equations are split into a left-hand side $f_i(\phi)$ and a right-hand side $g_i(\phi)$. When relaxation does work, it is slow to converge. In particular the long wavelength features of the solution must slowly "diffuse" across the grid with successive relaxation sweeps.

To solve a problem with multigrid methods we introduce a hierarchy of grids with different resolutions. For the moment, consider the case in which we seek the numerical solution of an elliptic equation on a uniform grid of size N^3 that covers the entire computational domain. We introduce grids of size $(N/2)^3$, $(N/4)^3$, etc., each covering the computational domain. On each grid the finite difference equation, or an associated equation, is solved by relaxation. The equations to be solved on each multigrid level are discussed in Section 4. For now, we simply note that the equations are chosen so that relaxation on the coarse grids quickly captures the long wavelength features of the solution. Relaxation on the fine grids captures the short wavelength features. The grids in the multigrid hierarchy communicate with one another through restriction and prolongation operators. Restriction takes data on a grid in the hierarchy and restricts it to the next coarsest grid. Prolongation takes data on a grid in the hierarchy and interpolates it onto the next finest grid. Different multigrid algorithms use different sequences of grids in solving elliptic problems, but the most basic sequence is the V-cycle. In a multigrid V-cycle one starts with the finest grid, steps down the grid hierarchy to the coarsest grid, then steps back up to the finest grid.

In the context of a time-dependent problem, adaptive mesh refinement (AMR) means that the grid structure adapts in time to meet the changing demands as the fields evolve. In the context of an elliptic (timeindependent) problem, AMR means that the grid structure is determined adaptively, as part of the solution process, in an attempt to minimize numerical errors.

We use the Paramesh package to organize the grid structure for our code. Paramesh covers the computational domain with blocks of data of varying spatial resolution. These blocks form a tree datastructure. They are logically Cartesian, consisting of a fixed number of cells. We typically use 8³ cells for each block. Fig. 1 shows an example one-dimensional grid. The numbers in that figure indicate the resolution level, and the letters denote blocks. At the base of the tree structure is a single block, labeled 1A. Paramesh refines blocks by bisection in each coordinate direction. In this one-dimensional example block 1A is refined into two blocks, 2A and 2B. Since each data block contains the same number of cells, level 2 has twice the resolution as level 1. Using Paramesh terminology, block 1A is the "parent" of blocks 2A and 2B, and blocks 2A and 2B are the "children" of block 1A. In Fig. 1 Paramesh has



Fig. 1. Example of a one-dimensional grid structure. The numbers on the left denote the resolution level, and the letters label blocks of data.

also refined blocks 2A and 2B to create blocks 3A, 3B, 3C and 3D. Further refinements yield the nonuniform grid shown in the figure. Paramesh always creates grid structures in which adjacent blocks' refinement levels differ by no more than one.

Our first task is to decide how to carry out a basic multigrid V-cycle on a non-uniform grid structure. There are two natural approaches. The first approach is the fast adaptive composite grid method (FAC) developed by McCormick [31]. In this approach, the relaxation sweeps extend across the entire computational domain, and one defines the succession of multigrid levels by restricting the highest resolution subgrid to the next lower resolution. As an example based on Fig. 1, we let the top multigrid level consist of blocks 4A-5A-5B-5C-5D-4D-3C-4E-4F. After carrying out a series of relaxation sweeps on this non-uniform grid, we step down the multigrid level by restricting the data in blocks 5A-5B-5C-5D to resolution level 4. Thus, the next multigrid level is defined by blocks 4A-4B-4C-4D-3C-4E-4F. After relaxing on this grid, we restrict the resolution level 4 blocks to resolution level 3. This defines the next multigrid levels, each covering the entire computational domain.

The second approach, the one we use for AMRMG, is to define the grids in the multigrid hierarchy to coincide with the different resolution levels. This is the original multi-level adaptive technique (MLAT) proposed by Brandt [25,32]. As an example based on Fig. 1, the top multigrid level consists of all blocks at resolution level 5, namely, 5A-5B-5C-5D. After carrying out a series of relaxation sweeps on the level 5 blocks, we restrict that data to level 4. Then the next multigrid level consists of blocks 4A-4B-4C-4D-4E-4F. After relaxing on these blocks we restrict the resolution level 4 data to resolution level 3. Then the next multigrid level consists of the level 3. Then the next multigrid level consists of the level 3 blocks 3A-3B-3C-3D. We continue in this fashion to define a complete multigrid hierarchy.

We have built and tested a one-dimensional multigrid code based on the FAC approach. That code works quite well. However, the MLAT approach appeared to us to be more straightforward to implement in a three-dimensional code based on Paramesh. For this reason AMRMG defines the levels in the multigrid hierarchy by resolution. Apart from the issue of implementation, the MLAT approach has an advantage in solving problems in which only a small region of the computational domain requires high resolution. With the FAC approach, in which relaxation always extends across the entire computational domain, a lot of unnecessary computational effort can be expended on relaxation in the low resolution regions. On the other hand, the FAC approach has the advantage over MLAT in maintaining a tighter coupling between regions of different resolutions. For example, for the grid shown in Fig. 1, the data in blocks 4A and 4D effectively provide boundary conditions for relaxation in blocks 5A through 5D. With FAC, that boundary information is updated between every relaxation sweep across the top multigrid level (4A–5A-5B-5C-5D-4D-3C-4E-4F). With MLAT, in which the top multigrid level consists of blocks 5A-5B-5C-5D, the boundary information is only updated once each V-cycle.

3. Guard cell filling

AMRMG uses cell centered data. When we apply the relaxation formula $f_i(\phi^{\text{new}}) = g_i(\phi^{\text{old}})$ to a cell adjacent to a block face, the finite difference stencil extends beyond the block. Paramesh uses layers of guard cells surrounding each block to hold data from beyond the block boundaries. In Fig. 2, we show a portion of a one-dimensional grid with a fine grid block on the left and a coarse grid block on the right. The grid points are labeled by their distance from the block interface in units of the fine grid cell size Δx . Thus, the fine grid points are -1/2, -3/2, etc., and the coarse grid points are 1, 3, etc. The gray circle at location +1/2 is a guard cell for the fine grid block, and the gray square at location -1 is a guard cell for the coarse grid block. Guard cell values are obtained by interpolation from surrounding interior data points. We want to consider how errors in guard cell filling affect the accuracy of the solution.

Consider the simple example of the Poisson equation in one-dimension, $\partial^2 \phi / \partial x^2 = \rho$. For the moment let us consider a uniform numerical grid with grid spacing Δx . With standard second order centered differencing, the discrete Poisson equation is

$$\frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2} + \mathcal{O}(\Delta x^2) = \rho_i,\tag{1}$$

where *i* labels the grid points. The term $\mathcal{O}(\Delta x^2)$ is the truncation error obtained from discretization of the second derivative. We can rewrite Eq. (1) in a form appropriate for relaxation as

$$\phi_i^{\text{new}} = \frac{1}{2} (\phi_{i+1}^{\text{old}} + \phi_{i-1}^{\text{old}}) - \frac{1}{2} \Delta x^2 \rho_i + \mathcal{O}(\Delta x^4).$$
(2)

When we apply this relaxation formula, the truncation error dictates that the numerical solution will have errors of order Δx^2 . That is, the numerical solution will be second order accurate.

For the non-uniform grid of Fig. 2, the discrete equation (1) and the relaxation formula (2) apply as shown in the fine grid region, where i = -1/2, -3/2, etc. For relaxation at the grid point i = -1/2, we need the guard cell value $\phi_{1/2}$. We want the guard cell value to be sufficiently accurate that it does not spoil the second order convergence of the solution. It is clear from these equations that errors of order Δx^4 in the value of $\phi_{1/2}$ can be absorbed into the truncation error already present. Thus, we expect the numerical solution to be second order convergent if the guard cells are filled to fourth (or higher) order accuracy.

As far as we know, fourth order guard cell filling is *sufficient* to produce a second order accurate solution for second order partial differential equations discretized on a non-uniform grid with standard second order differencing. Fourth order guard cell filling, however, is not a *necessary* condition. There is a "rule of thumb" in the computational mathematics community that can be summarized as follows [32,33,26]: errors of order Δx^p that occur on a subspace of dimension *m* in a space of dimension *n* will often contribute to the solution like errors of order Δx^{p+n-m} from the bulk. Thus, we anticipate that errors of order Δx^3 in guard

Fig. 2. A portion of a one-dimensional grid, showing three cells from a fine grid block on the left and two cells from a coarse grid block on the right.

cell filling, which occur on the two-dimensional block boundaries in the three-dimensional space, will contribute like errors of order Δx^4 from the bulk and will not spoil the second order convergence of our code. For the problems that we have studied this is indeed the case.

The guard cell filling scheme that we use was written by Kevin Olson as part of the standard Paramesh package. The process of filling the guard cells of a fine grid block that is adjacent to a coarse grid block proceeds in two steps. The first step is a restriction operation in which cells from the interior of the fine grid block are used to fill the interior cells of the underlying "parent" block. The restriction operation is depicted for the case of two spatial dimensions in the left panel of Fig. 3. The restriction proceeds as a succession of one-dimensional quadratic interpolations, and is accurate to third order in the grid spacing. Note that the fine grid stencil used for this step (nine black circles in the figure) cannot be centered on the parent cell (gray square). In each dimension the stencil includes two fine grid cells on one side of the parent cell and one fine grid cell on the other. The stencil is always positioned so that its center is shifted toward the center of the block (assumed in the figure to be toward the upper left). This ensures that only interior fine grid points, and no fine grid guard cells, are used in this first step.

For the second step, the fine grid guard cells are filled by prolongation from the parent grid. Before the prolongation, the parent block gets its own guard cells (black squares in the right panel of Fig. 3) from the neighboring block at the same refinement level. The stencil used in the prolongation operation is shown in the right panel of Fig. 3. The prolongation operation proceeds as a succession of one-dimensional quadratic interpolations, and is third order accurate. In this case, the parent grid stencil includes a layer of guard cells (black squares), as well as its own interior grid points (gray squares). At the end of this second step the fine grid guard cells are filled to third order accuracy.

When Paramesh fills the guard cells of a parent block, it also fills the guard cells of the parent's neighbor at the same refinement level. In Fig. 3, the parent's neighbor is the coarse grid block on the right side of the refinement boundary. Since we are using the second approach to multigrid outlined in Section 2, we do not relax in the parent's neighbor block until we step down the multigrid hierarchy. Thus, the guard cell values assigned to a parent's neighbor by the Paramesh guard cell filling routine are not used by AMRMG.



Fig. 3. The picture on the left shows the first step in guard cell filling, in which one of the parent grid cells (gray square) is filled using quadratic interpolation across nine interior fine grid cells (black circles). The other parent grid cells are filled using corresponding stencils of nine interior fine grid cells. The picture on the right shows the second step in which two fine grid guard cells (gray circles) are filled using quadratic interpolation across nine parent grid values (squares). These parent grid values include one layer of guard cells (black squares) obtained from the parent's neighbor on the right side of the interface, and two layers of interior cells (gray squares).

4. The FAS algorithm

AMRMG uses the full approximation storage (FAS) multigrid algorithm [25,34]. In this section, we provide a brief overview of FAS, and discuss the order of restriction and prolongation operators used for stepping down and up the multigrid hierarchy.

We are interested in the nonlinear elliptic differential equation $E(\cdot) = \rho$, where *E* is a (possibly) nonlinear elliptic operator. To avoid confusion with notation for exact and approximate solutions, we use a centered "dot" as a placeholder for the unknown function. Now consider a simple multigrid hierarchy consisting of two grids, a fine grid at level 2 and a coarse grid at level 1. The differential equation $E(\cdot) = \rho$, discretized on the finest level, becomes $E_2(\cdot) = \rho_2$. Here, the subscripts denote the multigrid level. What we seek is a solution of the difference equations $E_2(\cdot) = \rho_2$.

The basic V-cycle for the FAS algorithm consists of the following steps.

Step 1. Guess a trial solution $\tilde{\phi}_2$ (for example, $\tilde{\phi}_2 = 0$) and carry out some number of relaxation sweeps on the equation $E_2(\cdot) = \rho_2$ to obtain an approximate solution ϕ_2 .

Step 2. Construct the coarse grid source

$$\rho_1 = \mathscr{R}(\rho_2 - E_2(\phi_2)) + E_1(\mathscr{R}\phi_2). \tag{3}$$

Here, \mathscr{R} denotes the restriction of data from multigrid level 2 to level 1. Also, E_1 denotes the discretization of the elliptic operator E on the coarse grid 1. Loosely speaking, the term $-\mathscr{R}(E_2(\phi_2))$ removes the predominantly short wavelength part of the source that the fine grid has already captured in Step 1. The term $E_1(\mathscr{R}\phi_2)$ returns the long wavelength part of the source that was removed by subtracting $\mathscr{R}(E_2(\phi_2))$.

- Step 3. Start with the trial solution $\tilde{\phi}_1 = \Re \phi_2$ and carry out some number of relaxation sweeps on the equation $E_1(\cdot) = \rho_1$ to obtain an approximate solution ϕ_1 . Alternatively, if possible, solve $E_1(\cdot) = \rho_1$ exactly for ϕ_1 .
- Step 4. Construct the trial solution

$$\phi_2 = \phi_2 + \mathscr{P}(-\mathscr{R}\phi_2 + \phi_1). \tag{4}$$

Here, \mathscr{P} denotes the prolongation of data from multigrid level 1 to level 2. Loosely speaking, the term $\mathscr{P}(-\mathscr{R}\phi_2 + \phi_1)$ removes the long wavelength part of ϕ_2 and replaces it with ϕ_1 , which contains primarily long wavelength information due to the construction of ρ_1 .

Step 5. Start with the trial solution ϕ_2 from Step 4 and carry out some number of relaxation sweeps on the equation $E_2(\cdot) = \rho_2$ to obtain an improved approximate solution ϕ_2 .

For successive V-cycles the approximate solution ϕ_2 from Step 5 is used as the trial solution ϕ_2 in Step 1. The FAS V-cycle can be generalized in an obvious way to any number of multigrid levels.

At the bottom of each V-cycle Step 3 instructs us to find an exact or approximate solution of the equation $E_1(\cdot) = \rho_1$. The subscript '1' denotes the coarsest level in the multigrid hierarchy. It is important for the performance of any multigrid code to solve this equation accurately. Solving the level 1 equation can be a potential bottleneck for our code because Paramesh places the data for each block on a single processor. When the algorithm is at the bottom of a V-cycle, only a single processor is active.

The simplest strategy for solving the level 1 equation $E_1(\cdot) = \rho_1$ is to carry out relaxation sweeps, just as we do for the higher multigrid levels. Typically our coarsest multigrid level is a single data block with 8³ interior grid points. We find that with Robin boundary conditions it typically takes about one hundred relaxation sweeps to solve the level 1 equation to sufficiently high accuracy. With fewer sweeps at this level the code can require more V-cycles to solve the elliptic problem.

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The concern is that the solution of the level 1 equation, requiring ~ 100 sweeps with only one processor active, can dominate the run time for the code. However, it turns out that the run time for AMRMG is dominated by communications calls made in Paramesh. Currently AMRMG uses version 3.0 of Paramesh, which is one of the first versions of Paramesh to run under MPI. More recent versions are better optimized, but we have not switched to the latest version of Paramesh because of the special modifications that AMRMG requires.

One way that we have improved the performance of our code is to bypass the communications calls made by Paramesh when solving the level 1 equation. The data for the level 1 equation always resides on block #1 on processor #1, so no communication among processors is needed. We have bypassed the Paramesh guard cell filling routine by writing a routine that directly fills the guard cells of this block using the outer boundary conditions.

We are primarily interested in solving elliptic problems that are semi-linear, that is, problems in which the second order derivative terms are linear in the unknown field. For these problems the equation to be solved at the bottom of each V-cycle takes the form $\Delta_1\phi_1 = \rho_1$, where Δ_1 is the Laplacian operator (not necessarily on flat space with Cartesian coordinates) discretized on multigrid level 1. In these cases we have an alternative to relaxation, namely, direct matrix inversion: $\phi_1 = (\Delta_1)^{-1}\rho_1$. We have implemented matrix inversion for level 1 using the direct Gaussian elimination routine from the LAPACK libraries [35]. With Robin boundary conditions, we must solve the level 1 equation for ϕ values in the guard cells as well as interior cells. With 8³ interior grid points and one layer of guard cells, we have 10^3 values to determine at the bottom of each V-cycle. Therefore the matrix to be inverted has dimensions 1000×1000 . Our tests show that it takes longer (by a factor of ~10) to solve the level 1 equation by direct matrix inversion than by relaxation, assuming the Paramesh communications calls have been bypassed. However, in either case the time required to solve the level 1 equation is a small fraction of the overall runtime for the code. Thus, we prefer to use the direct matrix inversion whenever possible because, with matrix inversion, the accuracy of the level 1 solution is insured.

5. Restriction and prolongation

As described in Section 3, guard cells are filled with a combination of restriction and prolongation operations. The operators used for guard cell filling are third order accurate, and we denote these by ${}^{(3)}\mathcal{R}$ for restriction and ${}^{(3)}\mathcal{P}$ for prolongation. What order restriction and prolongation operators do we use for stepping down and up the multigrid hierarchy? The answer is that we use a combination of second, third, and fourth order operators.

The restriction operators in Paramesh are always defined in such a way that only interior cells from the child blocks are used to fill the interior cells of a parent block. The fine grid stencil is positioned to keep the coarse grid point as close as possible to the center of the stencil. For the case of second order restriction, ${}^{(2)}\mathcal{R}$, the coarse grid point lies at the center of the stencil and gets its value from a succession of linear interpolations in each dimension. The case of third order restriction, ${}^{(3)}\mathcal{R}$, is depicted in the left panel of Fig. 3 and is described in Section 3.

The second, third, and fourth order prolongation operators in Paramesh use a succession of (respectively) linear, quadratic, and cubic interpolations in each dimension to fill the fine grid cells. The prolongation operators use both interior cells and guard cells from a parent block to fill both interior and guard cells of child blocks. The right panel of Fig. 3 shows the stencil used by the third order prolongation operator, ${}^{(3)}\mathcal{P}$, to fill fine grid guard cells on the right side of a fine grid block. This same stencil is used to fill the first layer of interior cells (the layer of interior fine grid cells adjacent to the block boundary). For the second and third layer of interior fine grid cells, the stencil is shifted to the left by one coarse grid point. This pattern of stencil shifting continues across the right half of the fine grid block until the midpoint of the block is reached. The stencils used for the left half of the fine grid block are the mirror images of those used for the right half.

The version of Paramesh currently used by AMRMG allows for second and third order restriction, and (in principle) arbitrary order prolongation. We have carried out many numerical tests to help us choose among different combinations of restriction and prolongation operators for stepping down and up the V-cycles. For all of these tests we used third order restriction and third order prolongation to fill the fine grid guard cells, as described in Section 3. In our tests we did not consider prolongation orders higher than four.

As we have presented it, the FAS algorithm uses two restriction operators in Step 2, one restriction operator in Step 3, and one restriction operator in Step 4. It uses one prolongation operator in Step 4. One could consider distributing the (assumed linear) restriction operator through the first term in Eq. (3) and treating the operators independently. Likewise, one could consider distributing prolongation operator through the second term in Eq. (4) and treating the operators independently. We have not considered the consequences of splitting these terms. Moreover, AMRMG is written such that the calculation $\Re \phi_2$ from Step 2 is used as the trial solution $\tilde{\phi}_1 = \Re \phi_2$ for Step 3. Thus, we have not tested the consequences of treating these restriction operators independently. Note that the restriction of the fine grid solution, $\Re \phi_2$, appears in Step 4 as well as Steps 2 and 3. Our tests show that the order of the restriction operator in Step 4 must agree with the order used for $\Re \phi_2$ in Steps 2 and 3. If not, the algorithm will often fail to converge in the sense that the residual (defined below) will not decrease with successive V-cycles.

The options that remain for restriction and prolongation operators can be expressed by rewriting Eqs. (3) and (4):

$$\rho_1 = {}^{(b)} \mathscr{R}(\rho_2 - E_2(\phi_2)) + E_1({}^{(a)} \mathscr{R}\phi_2), \tag{5a}$$

$$\tilde{\phi}_2 = \phi_2 + {}^{(c)} \mathscr{P}(-{}^{(a)} \mathscr{R} \phi_2 + \phi_1).$$
 (5b)

The letters *a*, *b*, and *c* represent the orders of restriction and prolongation operators that appear in stepping down and up the V-cycles.

We want to find values for *a*, *b*, and *c* that will give the best performance. In judging the performance of our code we are looking to see how quickly the residual decreases with successive V-cycles for a fixed nonuniform mesh. The residual at each point in the computational domain is defined by res = $\rho_n - E_n(\phi_n)$, where *n* is the highest refinement level at that point and ϕ_n is the approximate solution. The norm of the residual is computed as

$$\langle \operatorname{res} \rangle = \sqrt{\frac{1}{N} \left(\sum \operatorname{res}^2 \right)}.$$
 (6)

The sum extends over the grid points that cover the computational domain at the highest refinement level. (In Fig. 2 these would be the interior points of blocks 4A-5A-5B-5C-5D-4D-3C-4E-4F.) The number N is the total number of such grid points. The norm (res) defined above is similar to the usual L_2 norm, but lacks a factor of the cell volume in the "measure" of the sum. That is, the usual L_2 norm would be written as $\sqrt{(\sum v res^2)/V}$, where v is the volume of each grid cell and V is the total volume of the computational domain. By omitting the factors of cell volume, the norm (res) gives equal weighting to the residuals in each grid cell, regardless of resolution.

To be specific, we will quote the results for the simple test problem $\Delta \phi = \rho$, where Δ is the flat space Laplacian in Cartesian coordinates. We use the source $\rho = (6 - 9r^3)\exp(-r^3)$ with $r = \sqrt{x^2 + y^2 + z^2}$. At the boundaries we use the Robin condition $\frac{\partial}{\partial r}[r(\phi - 1)] = 0$. The analytic solution to this problem is $\phi = 1 + (1 - \exp(-r^3))/r$. The numerical solution is computed with a fixed three-level "box-in-box" grid structure. The highest resolution region has cell size $\Delta x = 0.125$ and covers a cubical domain with x, y, and z ranging from -2 to 2. The medium resolution region has cell size $\Delta x = 0.25$. It covers the domain from

-4 to 4 that is exterior to the high resolution region. The low resolution region has cell size $\Delta x = 0.5$. It covers the domain from -8 to 8 that is exterior to the medium resolution region. It has been our experience that the generic behavior of AMRMG is fairly well represented by this simple test case.

Our first observation is that with a = 2 the residual gets "stuck" after a few V-cycles. The norm (res) drops to about 10^{-4} , but no further. This happens regardless of the values chosen for b and c. In the limit of high resolution the truncation error is less than the residual, and the code fails to show second order convergence of the solution. Thus, we can eliminate the cases in which a = 2 and focus on a = 3.

For a = 3 the norm of the residual decreases with successive V-cycles to values well below the truncation error. Table 1 shows the average change in the common logarithm of $\langle \text{res} \rangle$ for each V-cycle, as a function of the number of relaxation sweeps at each multigrid level. (This excludes the first multigrid level, at the bottom of each V-cycle, where we compute the exact solution using matrix inversion.) The best performance is obtained with (a, b, c) = (3, 2, 4). Note that the norm of the residual becomes insensitive to the number of relaxation sweeps as the number of sweeps increases beyond four or five. This is because, as observed in Section 2, the higher multigrid levels that have lower resolution neighbors can only receive updated boundary information once each V-cycle. It does not help to continue relaxation sweeps when the boundary information is "old" and needs to be updated. We typically use four relaxation sweeps, with red-black Gauss–Seidel ordering [34].

The results of our testing lead to the following formulas for Steps 2 and 4 of the FAS algorithm:

$$\rho_1 = {}^{(2)}\mathscr{R}(\rho_2 - E_2(\phi_2)) + E_1({}^{(3)}\mathscr{R}\phi_2), \tag{7a}$$

$$\tilde{\phi}_2 = \phi_2 + {}^{(4)}\mathscr{P}(-{}^{(3)}\mathscr{R}\phi_2 + \phi_1).$$
(7b)

In Step 3, we use the trial solution $\tilde{\phi}_1 = {}^{(3)} \mathscr{R} \phi_2$. Recall that we have not tested the algorithm with order of restriction greater than 3, or with order of prolongation greater than 4.

Conventional wisdom for determining the orders of restriction and prolongation used for multigrid transfer operations is that the following should be satisfied:

$$\mathcal{O}_{\mathscr{R}} + \mathcal{O}_{\mathscr{P}} > \mathcal{O}_{\mathscr{Q}}. \tag{8}$$

Here, $\mathcal{O}_{\mathscr{R}}$, $\mathcal{O}_{\mathscr{P}}$, and $\mathcal{O}_{\mathscr{D}}$ are the orders of restriction, prolongation, and the differential operator, respectively [36]. For a uniform grid, AMRMG acts as a typical FAS multigrid solver and we achieve acceptable convergence rates as long as the transfer operators satisfy Eq. (8). With a nonuniform grid, the restriction operator denoted ^(a) \mathscr{R} in Eqs. (5) must be third or higher order, at least in the vicinity of mesh refinement boundaries, for the code to achieve both second order accuracy and optimal convergence rates. This is not surprising since, with the MLAT approach, data that is restricted from a high resolution region (for example, data restricted from block 5D to block 4C in Fig. 1) can serve as boundary data for relaxation in a coarse grid region (block 4D in Fig. 1). With restriction order less than 3, such boundary data yield truncation errors greater than $\mathscr{O}(\Delta x)$ when they appear in a discrete second derivative. One of our goals

| Table 1 | | | | |
|---------|-----------|----------------------------|-----|---------|
| Average | change in | $log(\langle res \rangle)$ | per | V-cycle |

| Number of sweeps | Order of restriction and prolongation operators (a, b, c) | | | | | | | |
|------------------|---|---------|---------|-----------|---------|---------|--|--|
| | (3,2,2) | (3,2,3) | (3,2,4) | (3, 3, 2) | (3,3,3) | (3,3,4) | | |
| 1 | -0.00 | -0.11 | -0.16 | -0.11 | -0.13 | -0.33 | | |
| 2 | -0.32 | -0.42 | -0.50 | -0.33 | -0.46 | -0.56 | | |
| 3 | -0.56 | -0.75 | -0.77 | -0.43 | -0.56 | -0.69 | | |
| 4 | -0.77 | -0.88 | -1.13 | -0.50 | -0.63 | -0.74 | | |
| 5 | -0.85 | -1.08 | -1.21 | -0.56 | -0.68 | -0.79 | | |
| 6 | -0.87 | -1.15 | -1.23 | -0.62 | -0.74 | -0.83 | | |

for AMRMG is to achieve second order accuracy and good convergence rates with minimal modification of the existing Paramesh framework. For this reason we have not explored the possibility of using modified finite difference stencils or modified transfer operators in the vicinity of mesh refinement boundaries.

6. Truncation error and grid control

AMRMG adapts the grid structure to the problem at hand in an attempt to keep the local truncation error under control. The local truncation error is defined across the computational domain on the grid that consists of the highest resolution blocks. In Fig. 2 these would be blocks 4A-5A-5B-5C-5D-4D-3C-4E-4F. Let us refer to this non–uniform grid as grid *h*. Then the local truncation error is defined by [25]

$$\tau_h = E_h(\phi|_h) - (E(\phi))|_h,\tag{9}$$

where ϕ is the exact solution of the continuum equation $E(\phi) = \rho$, and $\phi|_h$ is the projection of ϕ onto grid h. The discretization of the operator E on grid h is denoted by E_h . In a similar manner, we define the local truncation error τ_H on a grid H that is constructed from the parents of grid h blocks. Grid H covers the computational domain with half the resolution of grid h. The difference between the truncation errors on grids H and h is

$$\tau_H - \mathscr{R}\tau_h = E_H(\phi|_H) - (E(\phi))|_H - \mathscr{R}E_h(\phi|_h) + \mathscr{R}(E(\phi))|_h,$$

$$\tag{10}$$

where \mathscr{R} is a linear operator that restricts data from *h* to *H*. Let us assume that \mathscr{R} is third order accurate in the grid spacing. Then the second and fourth terms in Eq. (10) cancel to third order and, to this same order of accuracy, we find $\tau_H - \mathscr{R}\tau_h \approx E_H(\phi|_H) - \mathscr{R}E_h(\phi|_h)$.

The relative local truncation error is defined on grid H by [25]

$$\tau_h^H = E_H(\mathscr{R}\hat{\phi}_h) - \mathscr{R}(E_h(\hat{\phi}_h)),\tag{11}$$

where $\tilde{\phi}_h$ is the approximate numerical solution from grid *h*. Again we assume that the restriction operator is accurate to third order. Since the approximate solution coincides with the exact solution to leading order, $\tilde{\phi}_h \approx \phi|_h$, we see from Eqs. (10) and (11) that to leading order in the grid spacing the relative truncation error is related to the local truncation errors by $\tau_h^H \approx \tau_H - \Re \tau_h$. Since we use second order differencing for our elliptic problems the truncation errors are proportional to the square of the grid spacing. Then $\tau_H \approx 4\Re \tau_h$ and the relative truncation error is given by $\tau_h^H \approx 3\Re \tau_h$. This relation can be prolonged to the finest grid *h*, giving $\Re \tau_h^H \approx 3\Re \Re \tau_h$. The prolongation operator \Re , like the restriction operator \Re , is assumed to be third order accurate in the grid spacing. Then to third order accuracy $\Re \Re$ is the identity operator on *h*, and we have

$$\tau_h \approx \frac{1}{3} \mathscr{P} \tau_h^H. \tag{12}$$

Together, Eqs. (11) and (12) give

$$\tau_h \approx \frac{1}{3} \left({}^{(3)} \mathscr{P} E_H ({}^{(3)} \mathscr{R} \tilde{\phi}_h) - E_h (\tilde{\phi}_h) \right).$$
(13)

In AMRMG, we use this approximation of the local truncation error to monitor the errors and control the grid structure. Note that since the truncation error τ_h is proportional to the square of the grid spacing, the result (13) is valid to leading order only if third (or higher) order restriction and prolongation operators are used.

For the test problem described in Section 5, it is straightforward to calculate the analytic truncation error. Fig. 4 shows a comparison of the analytic truncation error with the computed approximation to



Fig. 4. Analytic truncation error and calculated truncation error along the z-axis.

the truncation error (13) for that test problem. The analytic truncation error is shown as a thick solid line, while the calculated truncation error is a thin line with filled circles.

In practice, we start the solution process by specifying a rather coarse grid structure, sometimes uniform sometimes not. The code V-cycles until the norm of the residual across grid h is less than the norm of the local truncation error across grid h. We write this as $\langle \operatorname{res} \rangle|_h < \langle \tau_h \rangle|_h$, where the norm of the truncation error is defined in the same way as the norm of the residual, Eq. (6). The code usually requires two or three Vcycles to meet this criterion. We then compute the norm of the truncation error $\langle \tau_h \rangle|_b$ for each block of grid h. Any block whose norm is greater than some threshold value, $\langle \tau_h \rangle|_b > \tau_{\max}$, is flagged for refinement. Paramesh rebuilds the grid structure and redistributes the data across processors. To obtain a trial solution in the newly formed blocks we prolong the solution from the parent blocks. The code then carries out V-cycles on this new grid structure with its new highest-resolution grid h. The entire process repeats until all blocks satisfy $\langle \tau_h \rangle|_b \leq \tau_{\max}$ and no blocks are flagged for refinement. At this point the code continues to V-cycle until two conditions are satisfied: (1) the norm of the residual in each block is less than the norm of the truncation error, $\langle \operatorname{res} \rangle|_b < \langle \tau_h \rangle|_b$; and (2) the norm of the residual across the entire grid is less than some threshold value, $\langle \operatorname{res} \rangle|_h < \operatorname{res}_{\max}$. If only the first condition is desired, we simply set $\operatorname{res}_{\max}$ to a very large value.

We have tested the code using second, third, and fourth order prolongation operators for the calculation of trial solutions in newly formed blocks. We find that none of these operators is consistently better than the others. The entire adaptive mesh, multigrid algorithm is not very sensitive to the order of prolongation used in this step. We typically use the fourth order operator ${}^{(4)}\mathcal{P}$.

The grid control scheme used by AMRMG works well. It insures that the truncation error in each block across the computational domain is uniformly low, less than τ_{max} , and that the errors coming from the residuals in each block are less than the truncation errors. The value chosen for τ_{max} depends on the problem being solved and the desired degree of accuracy.

7. Code tests

In this section, we present code tests to demonstrate second order convergence and the computational advantages of AMR. Fig. 5 shows a comparison of errors for the test case described in Section 5.



Fig. 5. Errors along the z-axis for AMR grid and uniform grids of various resolutions.

The analytical errors on the z-axis are plotted for an AMR grid and for uniform grids with resolutions at levels 4, 5, 6 and 7. (A grid with resolution level X is created by refining a single block X - 1 times. See Fig. 1.) For the AMR run we start with a uniform level 3 grid and set the refinement criterion for a maximum truncation error of $\tau_{max} = 0.001$ in each block. We also limited the highest resolution to level 7, so the truncation errors in some of the level 7 blocks reached as high as 0.007. The cell size for resolution level 4 is $\Delta x = 0.25$, and the cell size for resolution level 7 is $\Delta x = 0.03125$. The grid structure chosen by AMRMG for the AMR run is shown in Fig. 6.



Fig. 6. AMR grid structure in the x-y plane. Each square corresponds to a block of data containing 8³ computational cells.

Observe that the errors in each region of the AMR grid are comparable to the errors obtained with a uniform grid of the same resolution. For example, the errors in the level 7 region of the AMR solution (the region surrounding the origin) are slightly larger than the errors obtained from the uniform level 7 solution, and smaller than the errors obtained from the uniform level 6 solution. We also note that the savings in memory with AMR is profound; the AMR grid solution can be calculated on a single processor, while the level 7 uniform grid solution required 64 processors to handle the memory requirements.

As a test for second order convergence, we consider the initial data for a single black hole. Valid initial data must satisfy the constraint equations of general relativity. For a vacuum spacetime, the Hamiltonian and momentum constraints are given, respectively, by

$$R + K^2 - K_{ij}K^{ij} = 0 (14)$$

and

$$D_j(K^{ij} - g^{ij}K) = 0, (15)$$

where g_{ij} is the physical metric and g^{ij} is its inverse. Also, R is the scalar curvature, K_{ij} is the extrinsic curvature with trace $K = K_i^i$, and D_j is the covariant derivative associated with the spatial metric. These initial value equations must be rewritten as a well-posed elliptic boundary value problem. The standard techniques for rewriting the constraint equations are based on the York–Lichnerowicz conformal decomposition [13]. Following this approach, we assume that the physical metric g_{ij} is conformally related to a background metric \tilde{g}_{ij} ,

$$g_{ij} = \psi^4 \tilde{g}_{ij},\tag{16}$$

where ψ^4 is the conformal factor. The physical extrinsic curvature is written as

$$K_{ij} = \psi^{-2} \tilde{K}_{ij}.$$

In terms of these conformal variables, the Hamiltonian and momentum constraints read

$$8\tilde{\nabla}^2 \psi - \psi \tilde{R} + \psi^{-7} \left(\tilde{K}_{ij} \tilde{K}^{ij} - \tilde{K}^2 \right) = 0, \tag{18a}$$

$$\tilde{\nabla}_{i}(\tilde{K}^{ij} - \tilde{g}^{ij}\tilde{K}) = -4\psi^{-1}\tilde{K}\tilde{\nabla}^{i}\psi, \qquad (18b)$$

where $\tilde{\nabla}_i$ and \tilde{R} are the covariant derivative and scalar curvature associated with the background metric \tilde{g}_{ii} .

The "puncture method" [37] is a way of specifying black hole initial data on \mathbb{R}_3 . The background metric is chosen to be flat. The momentum constraint (18b) is solved analytically by [38]

$$\tilde{K}^{ij} = \frac{3}{2r^2} (P^i n^j + P^j n^i - (\tilde{g}^{ij} - n^i n^j) P^k n_k),$$
(19)

where P^i is the momentum of the black hole and n^i is the radial normal vector (in the flat background with Cartesian coordinates). Note that \tilde{K}_{ij} is traceless, $\tilde{K} = 0$. This expression (19) for \tilde{K}_{ij} can be generalized to include an arbitrary number of black holes with spin and momentum, but for simplicity we will use a single black hole with no spin for our test case. To complete the specification of initial data, we must solve the Hamiltonian constraint (18a) for the conformal factor ψ . With the puncture method, the solution ψ is split into a known singular term and a nonsingular term u:

$$\psi = u + \frac{m}{2|\vec{r}|}.\tag{20}$$

Here, *m* is the "bare mass" of the black hole and $|\vec{r}|$ is the coordinate distance from the origin. With the puncture method splitting of the conformal factor, the Hamiltonian constraint becomes

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$$\nabla^2 u + \beta (1 + \alpha u)^{-7} = 0, \tag{21}$$

where

$$\beta = \frac{1}{8} \alpha^7 \tilde{K}^{ij} \tilde{K}_{ij} \quad \text{and} \quad \alpha = \frac{2|\vec{r}|}{m}.$$
(22)

Eq. (21) is solved for the nonsingular function u on \mathbb{R}_3 with Robin boundary conditions $\frac{\partial}{\partial v}[r(\phi-1)]=0$.

For these tests we use a fixed mesh refinement (FMR) grid with an "X plus 3" (Xp3) structure. The terminology Xp3 means that the grid is composed of 4 refinement regions, with the coarsest part of the grid at level X and the finest part of the grid at level X + 3. The different levels are nested in a "box-in-box" fashion. The finest level, with resolution X + 3, extends from -2 to 2 in each coordinate direction. The level with resolution X + 2 covers the domain between -4 and 4, excluding the finest level. The level with resolution X + 1 covers the domain between -8 and 8 excluding the finer levels. The coarsest level, with resolution X, covers the domain between -16 and 16 excluding the finer levels.

For our test case we have chosen m = 1 and $P^i = (0, 0, 1)$. We solve Eq. (21) using the series of FMR grids 3p3, 4p3, 5p3, 6p3, and 7p3. Each successive FMR grid has the same boundaries and double the resolution of the previous grid. Fig. 7 shows a contour plot of the solution u in the y-z plane, obtained with the 6p3 grid.

Figs. 8 and 9 show the results of a three-point convergence test for data along the z axis. This data passes through the puncture (at the origin) where the solution u and its derivatives are changing most rapidly. The three-point convergence test is obtained by plotting the difference between solutions on successive FMR grids, multiplied by an appropriate power of 4. The top (red) curve shown in Figs. 8 and 9 is the difference between the solution u obtained on the $4p_3$ grid and the solution obtained on the $3p_3$ grid. The next curve is the difference between solutions on FMR grids $5p_3$ and $4p_3$, multiplied by 4. The third curve is the difference between solutions on FMR grids $6p_3$ and $5p_3$, multiplied by 16. Finally, the curve that has the most negative value at the origin in Fig. 9 is the difference between solutions on the FMR grids $7p_3$ and $6p_3$, multiplied by 64. One can see that the curves in Figs. 8 and 9 overlay one another in the limit of high resolution. This shows that the errors in AMRMG are second order in the grid spacing.



Fig. 7. Contour plot of the non-singular part of solution u.

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Fig. 8. Three point convergence test of puncture data.



Fig. 9. Three point convergence test of puncture data close to puncture.

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