Tips for implementing multigrid methods on domains containing holes

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Abstract
As part of our development of a computer code to perform 3D ‘constrained evolution’ of Einstein’s equations in 3+1 form, we discuss issues regarding the efficient solution of elliptic equations on domains containing holes (i.e., excised regions), via the multigrid method. We consider as a test case the Poisson equation with a nonlinear term added, as a means of illustrating the principles involved, and move to a ‘real world’ three-dimensional problem which is the solution of the conformally flat Hamiltonian constraint with Dirichlet and Robin boundary conditions. Using our vertex-centred multigrid code, we demonstrate globally second-order-accurate solutions of elliptic equations over domains containing holes, in two and three spatial dimensions. Keys to the success of this method are the choice of the restriction operator near the holes and definition of the location of the inner boundary. In some cases (e.g. two holes in two dimensions), more and more smoothing may be required as the mesh spacing decreases to zero; however for the resolutions currently of interest to many numerical relativists, it is feasible to maintain second-order convergence by concentrating smoothing (spatially) where it is needed most. This paper, and our publicly available source code, are intended to serve as semi-pedagogical guides for those who may wish to implement similar schemes.

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1. Introduction
Solving Einstein’s equation in 3+1 form [1, 2] requires that a set of elliptic (or quasi-elliptic) constraint equations be satisfied at all times. The Bianchi identities ensure that, given a set of initial data which analytically satisfy the constraints, the subsequent analytically evolved variables will also satisfy the constraints. In numerical solutions of Einstein’s equations, however, the constraints are not preserved exactly. Thus errors will arise as the simulation
proceeds, and the extent to which the numerical solutions actually reflect the true solutions of
the continuum equations is still an open area of research (e.g., [3–7]). Apart from the issue
of the accuracy of the solutions obtained, there is also the problem of numerical (in)stability,
which seems to be related to the lack of preservation of the constraints.

It has been observed for lower-dimensional computational relativity simulations [8–10]
that the use of ‘constrained evolution’ schemes, in which the constraint equations are satisfied
(to some fixed accuracy) at all timesteps, can offer better stability behaviour. Such schemes
have not yet received adequate attention in 3D simulations largely because of the costly nature
of solving the constraints at every timestep. We are among a set of researchers (e.g., [11–13])
intrigued in exploring the benefits of constrained evolution for 3D applications.

Our desire to solve the constraints at each timestep motivates us to develop a fast elliptic
solver with which to enforce the constraints, and we turn our attention to one of the most popular
methods currently in use: the multigrid method [14]. The multigrid method is particularly
attractive because it is an optimal method, i.e. it requires only $O(N)$ operations, where $N$
is the number of unknowns. Furthermore, the multigrid method is not especially difficult to
implement. (Although multidomain pseudospectral collocation methods [15, 16] also offer
very efficient solutions of elliptic problems, we focus on multigrid because of the relative ease
with which one can develop a multigrid code. It is not our intent in this paper to present
a comparison between multigrid methods and other numerical methods.) In the course of
developing our own implementation of the multigrid method containing holes (i.e., excised
regions), it came to our attention that some researchers consider it impossible, or at least
infeasible in practice, to obtain generic results which have everywhere the same order of
accuracy as the finite difference scheme employed, for domains containing holes, particularly
in three dimensions (specifically, that, using second-order-accurate difference stencils, one
could not generically obtain second-order-accurate multigrid solutions if part of the domain
was excised).

Since we expect to use exact, analytic data as an inner Dirichlet boundary condition (at
the surface of the hole), we believe it is not necessary to employ ‘sophisticated’ schemes such
as deferred correction [17], which can be used to achieve higher-order accuracy for various
boundary conditions. We are already aware that one can fairly easily obtain second-order
convergence using square (in 2D) or cubical (in 3D) excision regions in which the physical
domain of the hole is the same on all multigrid levels. However, we wish to apply our multigrid
code in situations where the shapes of the holes are more general (e.g., spherical holes). Thus
we are motivated to find a simple, robust method to handle the physical situations of interest
to us.

If the multigrid solver is to be used to provide initial data for a numerical evolution code,
the error of the initial solution need only be below the truncation error of the finite difference
scheme used for evolution [18]. Thus our pursuit of specifically second-order convergence for
the multigrid scheme might be regarded as unnecessary. Our motivation is partly to develop
a simple algorithm which nevertheless offers fast (better than first-order) convergence, and
partly because, given our exact Dirichlet conditions for the inner boundary, we simply expect
that it should not be difficult to obtain second-order convergence from the multigrid solver.

Although it is likely the case that some of the techniques presented here are known to
some specialists, we believe it is worthwhile to popularize the straightforward methods we
have used.

If we were applying a numerical method to a new physical system, we would want
to provide a full discussion of mathematical foundations, for issues such as existence and
uniqueness of the solutions. Since the use of finite difference techniques to solve the
constraint equations is by now a standard activity in relativity, and the properties of the
constraint equations are well known (for the Euclidean, constant-mean-curvature background and for the signs of the solutions we use in this paper [19–21]), we will focus our attention on the benefits of our multigrid implementation: second-order accuracy near the hole via a simple method, and the efficiency improvements afforded by concentrating smoothing near the hole and performing more smoothing sweeps during the pre-coarse-grid-correction (CGC) phase than during the post-CGC phase. The validity of our results will be established by demonstrating second-order convergence to known exact solutions as well as second-order behaviour in the truncation error.

The organization of this paper is as follows: we begin with an overview of the multigrid method. We then discuss some results obtained in two dimensions, which we then extend towards a more difficult equation in three dimensions, eventually demonstrating the method by solving the Hamiltonian constraint equation for a black hole (with additional matter) on a Euclidean background. Finally we share some ideas for more general applications, and we end with a summary of the main five ‘tips’ we have for others wishing to implement multigrid methods on domains with holes.

2. Overview of multigrid

The multigrid method, first introduced by Brandt [14], has received considerable attention in the literature, and is the subject of numerous papers, conferences, reviews and books (e.g., [22–27]). However, its application on domains with holes—or on domains with ‘irregular boundaries’ in general—has received only modest attention. The excellent works of Johansen and Colella [28] and Udaykumar et al [29] for cell-centred multigrid are notable exceptions. The ‘BAM’ code [30] is a notable introduction of the multigrid method in numerical relativity, and even features the ability to handle domains with multiples holes. (It does not employ the advances we describe in this paper, notably our method of obtaining second-order accuracy near the hole.) Despite this significant result, multigrid methods in numerical relativity remain as tools of only a few specialists. We thus thought it worthwhile to share our experiences and methods with vertex-centred multigrid with the numerical relativity community.

A simple algorithm to solve discretized elliptic equations is Gauss–Seidel relaxation [31]. This method works very poorly at high resolutions because it fails to operate efficiently on long-wavelength components of the error. However, it is extremely effective at eliminating short-wavelength components of the error, or in other words, at ‘smoothing’ the error. The multigrid scheme is essentially a clever means of eliminating successive wavelength components of the error via the use of relaxation on multiple spatial scales.

Here we give a very brief overview of the multigrid method, following the notes by Choptuik [32]. (Introductions to multigrid applications in numerical relativity are also found in Choptuik and Unruh [33] and Brandt [34].) We want to solve a continuum differential equation \( L u = f \), where \( L \) is a differential operator, \( f \) is some right-hand side and \( u \) is the solution we wish to obtain. We discretize this differential equation into a difference equation on some grid (or lattice) with uniform spacing \( h \):

\[
L^h u^h = f^h, \tag{1}
\]

where \( u^h \) is the exact solution of this discrete equation, and \( \lim_{h \to 0} u^h = u \). Rather than attempting to solve (1) directly via the costly operation of matrix inversion, we apply an iterative solution method. At any step in our iteration, we will have only an approximate solution \( \tilde{u}^h \approx u^h \), such that

\[
L^h \tilde{u}^h - f^h = \tilde{r}^h, \tag{2}
\]
where \( \tilde{r}^h \) is some small quantity called the residual. The variables \( u^h \) and \( \tilde{u}^h \) are related by

\[
u^h = \tilde{u}^h + v^h,
\]

where \( v^h \) is some correction term. In this iterative algorithm, we start with some guess \( \tilde{u}^h \) and try to bring it closer to \( u^h \) by applying some (approximate) correction:

\[
\tilde{u}^h_{\text{new}} := \tilde{u}^h_{\text{old}} + \tilde{v}^h.
\]

The remainder of the scheme involves making a choice of what to use for \( \tilde{v}^h \). A simple choice, called the linear correction scheme (LCS), can be used for linear operators \( L^h \). This method can then be extended to work with nonlinear operators via the full approximation storage (FAS) method, below.

### 2.1. Linear correction scheme (LCS)

For linear \( L \), we begin by substituting (3) into (1):

\[
L^h(\tilde{u}^h + v^h) = f^h.
\]

Then we use the linearity of \( L \):

\[
L^h \tilde{u}^h + L^h v^h = f^h,
\]

\[
L^h v^h = f^h - L^h \tilde{u}^h = -\tilde{r}^h.
\]

Consider a coarser-grid version of (7), in which we use a mesh spacing of \( 2h \):

\[
L^{2h} \tilde{v}^{2h} = -\tilde{r}^{2h}.
\]

Now we come to one of the ‘tricks’ of the multigrid method: instead of the coarser residual in equation (8), use

\[
\tilde{r}^{2h} = I_{2h} \tilde{r}^h,
\]

where \( I_{2h} \) is a restriction operator, which maps values from the fine grid to the coarse grid via some weighted averaging operation. We then have

\[
L^{2h} \tilde{v}^{2h} = -I_{2h} \tilde{r}^h.
\]

(Note the tilde on \( \tilde{v}^{2h} \), which denotes that this is not the exact \( \tilde{v}^{2h} \), because we use a residual restricted from the fine grid.) Equation (10) can be solved ‘exactly’ for \( \tilde{v}^{2h} \) because this is inexpensive to do on the coarse grid.

A second ‘trick’ is that, for our correction term \( \tilde{v}^h \) in our numerical update scheme (4), we do not directly solve equation (7), but instead we use \( \tilde{v}^h \) approximated from the coarser (2\( h \)) correction \( \tilde{v}^{2h} \):

\[
\tilde{v}^h = I_{h} \tilde{v}^{2h},
\]

where \( I_{h} \) is an interpolation or prolongation operator, which maps values from the coarse grid to the fine grid via an interpolation operation. Thus we use \( \tilde{v}^{2h} \) as a coarse grid correction (CGC) to \( \tilde{u}^h \):

\[
\tilde{u}^h_{\text{new}} := \tilde{u}^h_{\text{old}} + I_{2h} \tilde{v}^{2h}.
\]

In performing the restriction \( \tilde{r}^{2h} = I_{2h} \tilde{r}^h \), we are assuming that \( \tilde{r}^h \) is sufficiently smooth to be sensibly represented on the coarse grid (e.g., without aliasing effects). This implies that \( \tilde{u}^h \) also needs to be smooth for this restriction to produce meaningful results. Therefore, before each restriction operation, we apply a series of ‘smoothing sweeps’ to \( \tilde{u}^h \) in an effort to smooth the residual \( \tilde{r}^h \), using the efficient smoothing algorithm of Gauss–Seidel relaxation.
2.2. Full approximation storage method (FAS)

For nonlinear operators \( L^h \), we must modify the algorithm outlined above. Our implementation relies on the so-called alternative description of the FAS algorithm, which involves a notion of the truncation error \( \tau^{2h} \), defined on the coarse grid by

\[
\tau^{2h} \equiv L^{2h}u^h - f^{2h},
\]

where \( u \) is the exact solution to the continuum equation. The function \( \tau^{2h} \) can be regarded as a correction term which makes the finite difference equation produce the continuum solution:

\[
L^{2h}u^h = f^{2h} + \tau^{2h}.
\]

For general problems, the continuum solution \( u \) and truncation error \( \tau^{2h} \) may not be available; however, we may use an approximation to \( \tau^{2h} \) which is the relative truncation error between the coarse and fine grids, \( \tau^h \), given by

\[
\tau^h \equiv L^h I^h L^h u^h - I^h \tilde{L}^h u^h.
\]

Using this in (14) gives

\[
L^{2h} u^{2h} \approx f^{2h} + \tau^h,
\]

and it is this equation which we solve on the coarse grid.

To obtain the CGC to a fine grid solution, we substitute (15) into (16), obtaining

\[
L^{2h} u^{2h} - L^{2h} I^h \tilde{L}^h \tilde{u}^h = I^{2h} (f^h - L^h \tilde{u}^h),
\]

where the term \( I^h f^h \) on the right is introduced for \( f^{2h} \), in analogy with equation (8). By analogy to (10) in the LCS scheme, the term we should use for the CGC is (the part on the left-hand side of the previous equation, without the \( L \)):

\[
\tilde{u}^{2h} = u^{2h} - I^h \tilde{L}^h \tilde{u}^h.
\]

Thus we arrive at an update scheme of

\[
\tilde{u}^{\text{new}} := \tilde{u}^{\text{old}} + I^h (u^{2h} - I^h \tilde{L}^h \tilde{u}^h).
\]

Note that \( u^{2h} \) is the exact solution to (16), and can be obtained with little effort due to the low resolution on the coarse grid. (If there are more than two multigrid levels involved in the solution, then \( u^{2h} \) should be the best approximation \( \tilde{u}^{2h} \) obtained on the coarser grid.)

2.3. V-cycles and the full multigrid algorithm

Instead of using only two grids as described above, one could find the CGC to a fine grid problem by solving for a CGC from an even coarser grid, i.e., obtain \( \tilde{u}^{2h} \approx u^{2h} \) by finding \( u^{4h} \) (in which case the corresponding right-hand side is \( f^{4h} + \tau^{4h} \), where \( f^{4h} \equiv I^{4h} (f^{2h} + \tau^{2h}) \)).

One can imagine a hierarchy of multiple such grids, in which coarser grids provide CGCs for finer grids. The solution algorithm will then take the form of a V-cycle, in which we start with an initial guess on the fine grid, at multigrid level \( l_{\text{max}} \). Then we perform some number of smoothing sweeps and restrict the data to a coarser grid. We continue smoothing and restricting to coarser grids until we arrive at a grid coarse enough to solve the coarse-grid equation (16) ‘exactly’ (i.e., to some specified tolerance, such as machine precision), at minimal computational cost. This coarsest grid is at level \( l_{\text{min}} \). We then prolongate this solution to finer grids by performing a series of CGCs, with perhaps additional smoothing operations being performed before moving to each finer grid.

In addition, before starting a V-cycle from the finest grid, we can use an initial guess obtained from a prior solution at a coarser resolution. Doing this for each grid level results in
the full multigrid algorithm (FMA). We outline the FMA as follows, (using a notation where superscripts refer to multigrid levels, with \( l_{\text{min}} \) denoting the coarsest level, and \( l_{\text{max}} \) denoting the finest):

\[
\begin{align*}
\mathbf{u}^{l_{\text{min}}} &= \mathbf{u}_0 \quad &\text{// Initial guess, e.g. } \mathbf{u}_0 = 0 \\
\text{Solve } L_{l_{\text{max}}} \mathbf{u}^{l_{\text{min}}} &= \mathbf{f}^{l_{\text{min}}} \text{ ‘exactly’} \quad &\text{// or } \mathbf{u}_0 = 1 \\
\text{do } i = l_{\text{min}} + 1 \text{ to } l_{\text{max}} \\
&\quad \mathbf{u}^i = \mathbf{I}^i_{l-1} \mathbf{u}^{i-1} \quad &\text{// Initial guess for fine grid} \\
&\quad \text{do } m = i \text{ to } l_{\text{min}} + 1 \\
&\quad &\quad \text{Smooth (solve via Gauss–Seidel) at level } m \\
&\quad &\quad \quad f^{m-1} = I^{m-1}_m f^m + \tau^{m-1}_m \quad &\text{// Pre-CGC smooths} \\
&\quad &\quad \quad \tilde{u}^{m-1} = I^{m-1}_m \mathbf{u}^m \quad &\text{// Restrict to coarser grid} \\
&\quad &\quad \text{end do} \\
&\quad \text{Solve } L_{l_{\text{min}}} \mathbf{u}^{l_{\text{min}}} &= \mathbf{f}^{l_{\text{min}}} \text{ ‘exactly’} \\
&\quad \text{do } m = l_{\text{min}} + 1 \text{ to } l_{\text{max}} \\
&\quad &\quad \mathbf{u}^i := \mathbf{u}^i + I^m_{m-1} (\mathbf{u}^{m-1} - I^m_{m-1} \mathbf{u}^m) \quad &\text{// Apply CGC} \\
&\quad &\quad \text{Smooth at level } m - 1 \quad &\text{// Post-CGC smooths} \\
&\quad &\quad \text{end do} \\
&\quad \text{end do} \\
&\quad \text{// End V-cycle} \\
&\quad \text{// End FMA} \\
\end{align*}
\]

Thus we see that on all grids except the coarsest grid, we only smooth the error, and we solve the difference equation exactly only on the coarsest grid.

### 3. Solution of a nonlinear Poisson equation

Since we are interested in ultimately solving for the constraint equations in general relativity, we consider the Hamiltonian constraint in a conformally flat background geometry. This yields the Poisson equation with a pair of nonlinear terms added:

\[
\nabla^2 u(x, y, z) - K^2 u^5(x, y, z) + A^2 u^7(x, y, z) = f(x, y, z),
\]

where \( \nabla^2 \) is the usual Laplacian in Euclidean space. \( K^2 \) and \( A^2 \) are arbitrary positive real constants related to the rate of expansion for the 3-space for which (20) is the constraint equation. \( f(x, y, z) \) is related to the energy density in the 3-space, and can be chosen such that the resulting \( u(x, y, z) \) has a known (exact) form by which we can check our numerical results.

Rather than begin with this somewhat complicated equation, we begin by solving a slightly simpler-looking equation in two and three dimensions, in which the nonlinearity is of a quadratic form, as in

\[
\nabla^2 u(x, y, z) + \sigma u^2(x, y, z) = f(x, y, z),
\]

where \( \sigma (\in \mathbb{R}) \) is a tunable parameter which we typically set to \( \pm 1 \) (although there are good reasons to prefer \( -1 \) over \( +1 \); see footnote 1 regarding smoothing operations). We chose this equation not because of any particular physical relevance, but simply because it was the
equation used in the version of Choptuik’s 2D multigrid code [35], with which we had prior experience.

Before proceeding to 3D calculations, we will describe our implementation for solving a 2D version of (21). Due to memory limitations (and array-indexing limitations in many Fortran compilers), we can run our (nonparallel) 3D code only at much lower resolutions than we are able to achieve with the 2D code. Since some of the interesting features in the convergence studies appear only at very high resolutions in our 2D results, we first present our 2D scheme and the results yielded by it.

3.1. Two dimensions

Our starting point is a 2D FAS multigrid solver by Choptuik [35], which solves the equation

$$\frac{\partial^2}{\partial x^2} u(x, y) + \frac{\partial^2}{\partial y^2} u(x, y) + \sigma u^2(x, y) = f(x, y),$$

(22)
on a domain $\Omega$ with coordinate ranges [0, 0] to [1, 1], and subject to Dirichlet conditions at the outer boundary: $u(x, y)|_{\partial\Omega} = \text{const}$, and we choose this constant to be zero. The function $f(x, y)$ is chosen such that the solution is

$$u(x, y) = \sin(\pi l_x x) \sin(\pi l_y y),$$

(23)
where $l_x$ and $l_y$ are integers (which we set to unity for the cases presented in this paper). We also choose $\sigma = 1$. Choptuik’s form assumed a domain without holes, but we extend this to configurations with holes, and on these inner boundaries we also apply Dirichlet conditions, the values for which are discussed below.

The code uses a hierarchy of so-called ‘vertex-centred’ grids. Each grid at multigrid level $l$ is a square lattice having $2^l + 1$ grid points along each edge. The grids have uniform spacing $h_l = 2^{-l}$ in both $x$ and $y$ directions, and the grid points are denoted by indices $i$ and $j$ in the $x$ and $y$ directions, respectively, e.g., $u(ih_l, jh_l) \approx \tilde{u}_{i,j}$.

To Choptuik’s original code, we added features needed to handle the excision region. We also performed a few minor optimizations. At each grid point, we also store an integer code which denotes whether the point is a boundary point, an excised point, or an interior (or active) point. The set of all excised points is known as the excision mask or mask, and for the cases considered in this paper, we define the mask to be those points which are at a distance $r \leq r_{\text{mask}}$ from the centre of the grid, where $r_{\text{mask}}$ is a value of our own choosing. The outermost points of the mask are where the inner boundary conditions are applied; we refer to these points as ‘inner boundary points’. In addition to the single-hole case, we will consider the case of two holes, for which the excision regions will be points within the radius $r_{\text{mask}}$ from the centre of each hole.

**Boundary conditions.** We use Dirichlet boundary conditions at both the inner boundary (edge of the hole) and the outer boundary, and apply them on all grid levels. At the outer boundary, we simply set $\tilde{u}^h = 0$. At the inner boundary, we use the values of the exact solution, i.e., we set $\tilde{u}^h = u(x, y)$.

The inner boundary is given by the outer edge of the points comprising the excision mask; an example is shown in figure 1. Thus, in some sense these boundary points are not truly ‘excised’ since they have data on them. This has the consequence that the ‘size’ of the excision region (i.e., the area of the convex hull of the data points comprising the mask) on finer grids is always equal to or greater than the size of the excision region on coarser grids. This choice of the inner boundary, as being those points just inside a level surface instead of just outside it, is somewhat at variance from other excision schemes used in numerical relativity (e.g., [36]).
Our choice is not fundamentally based on physical or mathematical principles, and is thus somewhat arbitrary. However we find that this definition of the inner boundary appears to be a key to our results of second-order convergence: if we instead define inner boundary points to be those just beyond \( r = r_{\text{max}} \), then we do not obtain second-order convergence.

**Smoothing operations.** We use a typical ‘red-black’ Gauss–Seidel Newton iteration to smooth the error on each grid, in which we loop over all 'interior' points (i.e. nonexcised, nonboundary points) and apply the following two equations

\[
\begin{align*}
 r_{\text{GS}} &= h^{-2}(\tilde{u}_{i+1,j} + \tilde{u}_{i-1,j} + \tilde{u}_{i,j+1} + \tilde{u}_{i,j-1} - 4\tilde{u}_{i,j}) + \sigma \tilde{u}_{i,j}^2 - f_{i,j}, \\
 \tilde{u}_{i,j}^{\text{new}} &= \tilde{u}_{i,j}^{\text{old}} - \frac{r_{\text{GS}}}{2\sigma \tilde{u}_{i,j} - 4h^{-2}}.
\end{align*}
\] (24)

\[
\tilde{u}_{i,j}^{2h} = I_{k}^{2h} \tilde{u}_{h} = \frac{1}{2} \tilde{u}_{i,j}^{h} + \frac{1}{2} \left( \tilde{u}_{i+1,j}^{h} + \tilde{u}_{i-1,j}^{h} + \tilde{u}_{i,j+1}^{h} + \tilde{u}_{i,j-1}^{h} \right),
\] (26)

where \( i = 2I - 1 \) and \( j = 2J - 1 \). Along the outer boundary, we perform a simple copy operation, \( \tilde{u}_{i,j}^{2h} = \tilde{u}_{i,j}^{h} \). We use (26) for all restriction operations on interior grid points with

1. We note an example of the care that must be taken in any solution of a discretized problem. Convergence of the solution may be impossible to achieve; this may signal significant analytical defects in the formulation. If \( \tilde{u} > 0 \), then \( \sigma = -1 \) guarantees that the Jacobian \( 2\sigma \tilde{u} - 4/h^2 \) is nonzero (its inverse is nonsingular in equation (25)). Clearly, there are in principle situations with \( \sigma \tilde{u} > 0 \) where the Jacobian can vanish. Further, because the equations we wish to solve are nonlinear, zeros of the Jacobian depend on \( \tilde{u} \) and may occur at isolated spatial points. Further, because \( 2\sigma \tilde{u} \) is similar on all grids, but \(-1/h^2\) is resolution dependent, this problem can appear differently on different multigrid levels. It may be that a more sophisticated solver could integrate through those singular points, but we do not address this question here. Note that because \( \tilde{u}_{i,j} \) is near unity in the case of ‘sine’ data given by equation (23), this problem does not arise for \( \sigma = 1 \) for ‘sine’ data. Similar comments apply, of course, in the 3D case of equation (21).
one exception: we only use weighted restriction if none of the fine grid points used in the restriction operator are on or inside the boundary of the excised region; otherwise we use a ‘simple injection’ or ‘copy’ operation. This is illustrated in figure 2. In conjunction with our definition of the inner boundary location, this use of a ‘copy’ operation near the inner boundary is the central insight for preserving second-order accuracy near the excision region.

For the prolongation operator $I_{2h}^h$, we use simple bilinear interpolation.

3.1.1 2D results. One of the first things we note when graphing preliminary numerical solutions is that the solution error $e = u - \tilde{u}^h$ seems to be largest and ‘most in need of smoothing’ (i.e., having high-frequency components) in the immediate vicinity of the excision region, as shown in figure 3.

Thus we may perform only a few smooths on the entire grid and apply extra smoothing runs in an ‘extra smoothing region’ (ESR) around the excision region, such as that shown in
Figure 4. Left panel: schematic of a level = 4 grid (2^{level} + 1 grid points per side) showing excised points (X), normal interior points (N), boundary points (B) and the ESR, (E). In this case, the excision region has radius $r_{\text{mask}} = 0.129$. Right panel: convergence behaviour of equations (22)–(25) with and without the use of the ESR. Here we show the L2 norm of the solution error $e = u - \tilde{u}$. We assign the width of ESR to be level − 1 grid points on either side of the hole, and we smooth twice as often over the ESR as over the normal interior points. Since the error is concentrated near the hole, we see that using two pre- and post-CGC smooths with the ESR (i.e., using four smooths in the ESR, and two smooths elsewhere) offers a substantial improvement over the use of three pre- and post-CGC smooths over the whole domain. We see that at high resolutions (level = 9–11) the error begins to rise again. To obtain results in keeping with second-order convergence at resolutions up to level = 11, more work is required. The use of three pre- and post-CGC smooths with the ESR (i.e., six smooths in the ESR, and three elsewhere) produces results comparable to those obtained by using six pre- and post-CGC smooths over the whole domain; however, the former requires a fraction of the computational cost of the latter.

in the left panel of figure 4. In our implementation, we choose the width of the ESR to be a number of grid points which is one less than the current multigrid level number (e.g., on a level 4 grid, the ESR has a width of three grid points), and we smooth over the ESR twice as often as over the rest of the domain. We can compare the results of using the extra smoothing region to the results of smoothing over the entire domain. Such a comparison is shown in the right panel of figure 4.

Two holes. One of our principal applications for the multigrid solver will be to solve the constraint equations for binary black-hole spacetimes. Thus we do a check to make sure that, at least for the nonlinear Poisson equation, our general method properly handles domains with multiple holes. One such case is shown in figure 5.

There is a contrast between the relative importance of pre-CGC smoothing and post-CGC smoothing. Pre-CGC smoothing prepares the data in such a way that restriction will not produce aliasing errors, whereas post-CGC smoothing in the large part corrects for errors brought in via the use of (linear) interpolation. It seems plausible that the former case (pre-CGC) would require at least as much smoothing as the latter (post-CGC); we see evidence for this in the two-hole solutions, such as those used to produce figure 5. Again we are able to achieve second-order convergence, for instance with 1 V-cycle, 12 pre-CGC sweeps and no post-CGC sweeps, and with more effort: 5 V-cycles, 20 pre- and post-CGC sweeps, shown for comparison as a ‘perfect’ multigrid result.
3.2. Three dimensions

For solving equations in 3D, we proceeded in steps, performing a few test cases until arriving at a code which solves the Hamiltonian constraint in 3+1 general relativity.

The first test case is similar to the 2D case discussed above, i.e., we choose \( f(x, y, z) \) such that the exact solution to (21) is

\[
  u(x, y, z) = \sin(\pi l_x x) \sin(\pi l_y y) \sin(\pi l_z z),
\]

where \( l_x, l_y \) and \( l_z \) are integers which we set to unity. We excised a sphere of radius \( r_{\text{mask}} = 0.129 \), which is a value chosen simply to ensure that the size of the mask is different on different grid levels, i.e. to make the test slightly more difficult than if we had chosen a multiple of the mesh spacing. For the test case involving a sinusoidal solution (27), the results are very similar to those of the 2D case. Having verified that the multigrid solver could adequately handle such a system and achieve second-order accuracy, we proceeded to the next step.

The next test case involves an equation (20) which corresponds to the solution of the Hamiltonian constraint equation for the conformally flat spacetime system [37]:

\[
  \nabla^2 u = \frac{K^2 u^5}{u^5} + \frac{A^2}{a^2} = f,
\]
where $K^2$ and $A^2$ are arbitrary positive real constants related to the expansion rate of the 3-space, and $r$ is the usual radial coordinate. We adjust the matter source term $f(x, y, z)$ such that the continuum solution is

$$u(x, y, z) = 1 + 2M/r.$$  \hfill (29)

Here $r$ is the usual radial coordinate, and we choose $M = 1$. The excision region contains $r = 0$ and the function values in this region are not calculated. On the inner boundary (the boundary of the excision region), we use values of the continuum solution as Dirichlet conditions on only the finest grid, and on coarser grids, we use data copied or extrapolated from finer grid data. One can simply copy values from the fine grid to the coarse grid wherever the boundary points on the fine and coarse grids coincide. Wherever they do not coincide, i.e., wherever the coarse-grid boundary points are ‘interior’ to the fine grid boundary points, we find it quite adequate to use quadratic extrapolation (in one dimension) from the neighboring (nonexcised) fine grid points to obtain the value at the location of a coarse-grid boundary point. The results we obtain appear to be rather insensitive to the form of the extrapolation used (e.g., the shape of the stencil). The use of extrapolated fine-grid data is an important difference from the way inner boundary values are obtained in the 2D code, and does constitute a great improvement over the generic applicability of our method.

For the outer boundary in this case, we can either apply Dirichlet conditions using the continuum solution $u(x, y, z)$, or we can use a mixed boundary condition called the Robin condition. The Robin condition requires

$$\frac{\partial}{\partial r} \left[ r (u - 1) \right] = 0,$$  \hfill (30)

on the boundary. The Robin condition is the standard condition used in relativity when a solution with the form (29) is desired (see, e.g., [37]). However $M$ is not a known constant until the solution is known, so the condition which the solution (29) satisfies, namely (30), is implemented as the boundary condition.

There are several ways to implement the Robin condition. Rather than taking derivatives in the radial direction as required by (30), we follow Alcubierre [38] and instead take derivatives only in directions normal to the faces of our cubical domain. This approach is much simpler to implement than using radial derivatives. We implement this using first-order difference stencils; for the $+x$ face of the domain, at location $x_i$, the stencil is simply

$$\tilde{u}_{i,j,k} = 1 + \left( \tilde{u}_{i-1,j,k} - 1 \right) \frac{r_{i-1,j,k}}{r_{i,j,k}},$$  \hfill (31)

where $r_{i,j,k}$ is the radial distance to lattice location $(i, j, k)$. We have also implemented alternative stencils: second-order stencils in the normal direction and a first-order stencil in the radial direction.

**Smoothing operations.** We use a simple ‘red–black’ Gauss–Seidel Newton iteration to smooth the error, i.e.,

$$r_{GS} = h^{-2} (\tilde{u}_{i+1,j,k} + \tilde{u}_{i-1,j,k} + \tilde{u}_{i,j+1,k} + \tilde{u}_{i,j-1,k} + \tilde{u}_{i,j,k+1} + \tilde{u}_{i,j,k-1} - 6\tilde{u}_{i,j,k}) - K^2 \tilde{u}_{i,j,k} + A^2 \tilde{u}_{i,j,k} - f_{i,j,k},$$  \hfill (32)

$$\tilde{u}_{i,j,k} = \tilde{u}_{i,j,k} - \frac{r_{GS}}{-5K^2 \tilde{u}_{i,j,k} - 7A^2 \tilde{u}_{i,j,k} - 6h^{-2}}.$$  \hfill (33)

**Restriction and prolongation operators.** For the restriction operator $I_{2h}^h$, we use a weighted average which is defined via a $3 \times 3 \times 3$ stencil, with a weight of $1/8$ on the central point,
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of the Robin condition suggested by Alcubierre [38]. In fact, the two graphs we obtain lie on Dirichlet outer boundary condition and the ‘first-order perpendicular’ (FOP) implementation lines which run parallel to the line for second-order behaviour at high resolutions, for both the Hamiltonian constraint, equation (28), is given in figure 6. The left panel shows that we obtain a graph of the convergence behaviour for the solution of the conformally flat background points, then we use a simple copy instead of weighted restriction. As in the 2D case, if any of the find-grid points included in the weighting are inner boundary points, then we use a simple copy instead of weighted restriction.

For the prolongation operator $I_{2h}^h$, we use simple trilinear interpolation.

3.3. 3D results

A graph of the convergence behaviour for the solution of the conformally flat background Hamiltonian constraint, equation (28), is given in figure 6. The left panel shows that we obtain lines which run parallel to the line for second-order behaviour at high resolutions, for both the Dirichlet outer boundary condition and the ‘first-order perpendicular’ (FOP) implementation of the Robin condition suggested by Alcubierre [38]. In fact, the two graphs we obtain lie on

Figure 6. Convergence results for 3D solutions to (28) of the form $u = 1 + 2M/r$, for runs in which $A^2 = K^2 = 1$, $r_{min} = 3$, and $r_{max} = 1.29$, for a domain $[5, 5, 5]$ to $[5, 5, 5]$. Left panel: a logarithmic plot of the L2 norm of the solution error $e = u - \tilde{u}^h$, showing a comparison between outer boundary conditions. Using the ‘first-order perpendicular’ (FOP) implementation (31) of the Robin boundary condition (30), we obtain convergence results which lie on top of those obtained using a Dirichlet outer boundary condition (where the values of the continuum solution are supplied at the outer boundary). These results also run parallel to the line for perfect second-order behaviour. Right Panel: a logarithmic plot of $e$ itself, at the end of each V-cycle in the full multigrid algorithm. These results correspond to the ‘1 V, 3 Pre, 3 Post, Dirichlet’ case shown in the left panel; however, its shape is resolution dependent. This feature may arise from the use of the FOP condition.

1/16 on the centre of each face, 1/32 on the centre of each edge and 1/64 on each corner, i.e. [30]

\[
\tilde{u}^{2h}_{i,j,k} = I_{2h}^h \tilde{u}^h = \frac{1}{5} \left( \tilde{u}^h_{i,j,k} + \frac{1}{h} \left( \tilde{u}^h_{i+1,j,k} + \tilde{u}^h_{i-1,j,k} + \tilde{u}^h_{i,j+1,k} + \tilde{u}^h_{i,j-1,k} + \tilde{u}^h_{i,j,k+1} + \tilde{u}^h_{i,j,k-1} \right) \right)
\]

As in the 2D case, if any of the find-grid points included in the weighting are inner boundary points, then we use a simple copy instead of weighted restriction.

For the prolongation operator $I_{2h}^h$, we use simple trilinear interpolation.

\[
\tilde{u}^h_{i,j,k} = \frac{1}{5} \left( \tilde{u}^h_{i,j,k} + \frac{1}{h} \left( \tilde{u}^h_{i+1,j,k} + \tilde{u}^h_{i-1,j,k} + \tilde{u}^h_{i,j+1,k} + \tilde{u}^h_{i,j-1,k} + \tilde{u}^h_{i,j,k+1} + \tilde{u}^h_{i,j,k-1} \right) \right) \]

(34)

\[
\tilde{u}^{2h}_{i,j,k} = \frac{1}{5} \left( \tilde{u}^{2h}_{i,j,k} + \frac{1}{h^2} \left( \tilde{u}^{2h}_{i+1,j,k} + \tilde{u}^{2h}_{i-1,j,k} + \tilde{u}^{2h}_{i,j+1,k} + \tilde{u}^{2h}_{i,j-1,k} + \tilde{u}^{2h}_{i,j,k+1} + \tilde{u}^{2h}_{i,j,k-1} \right) \right)
\]

(34)

As in the 2D case, if any of the find-grid points included in the weighting are inner boundary points, then we use a simple copy instead of weighted restriction.
4. Towards more general applications

We have made use of a known exact solution in two key elements of this paper: (1) supplying values for Dirichlet conditions on the inner boundary and (2) calculating the solution error $e = u - \tilde{u}$ for measuring the accuracy and convergence of the code. Since we wish to use the multigrid solver for situations in which an exact solution is not known across the whole domain (such as in a solution for the conformal factor in a general binary black-hole spacetime), we describe here the modifications to the previous discussion in the absence of an exact solution.

In the 2D code we used the continuum solution to supply Dirichlet conditions on the inner boundaries of all multigrid levels; however, for the 3D code we only used the continuum solution on the finest grid, and then extrapolated or copied data from finer grids to coarser grids. (There was nothing about the 2D case that made extrapolation impossible; rather it was simply a later feature which was added to the more advanced 3D code.) Although we were able to employ this extrapolation effectively in the cases we tried—using a very simple, almost arbitrary, 1D extrapolation method—it may be that such a method would be unstable for certain classes of equations. Although we see no evidence for this, and given the generality of the multigrid method one may expect much of what is found in this paper to apply to other systems of interest. We cannot offer complete assurance that extrapolation will work for all elliptic systems.
The assumption that an exact value is known at points on the finest grid may not be appropriate for many of the solutions of interest to numerical relativists. One may encounter systems with Neumann or Robin conditions at the inner boundary. Although we have not considered such cases explicitly, we suggest straightforward differencing similar to the treatment of the Robin conditions we reported above.

When one cannot measure the accuracy of the code by calculating the solution error, one can still gain a measure of the convergence of the code by monitoring the relative truncation error $\tau_{h}^{2h}$. One should disregard values at points adjacent to inner boundary points, as these tend to be poorly defined and exhibit blow-up behaviour, but all other points are eligible for comparison. A plot of $\tau_{h}^{2h}$ at various grid levels for a 3D solution is shown in figure 7, demonstrating the strict second-order behaviour of the solution on two different domains.

5. Conclusions

We offer five tips for those who wish to implement 2D or 3D multigrid methods for domains with holes.

1. The first and most important tip is really twofold:
   - apply inner boundary conditions on points immediately interior to (rather than exterior to, as is often done) a spatial surface such as a circle or sphere of a given radius. This has the effect that the extent of excision region is smaller on coarser grids than on finer grids.
   - when performing restriction operations, use weighted restrictions on all interior points, except in cases where the weighted operator would include points where the inner boundary conditions are applied. For the latter cases, use a simple copy operation.

2. Concentrate smoothing operations where they are most needed. We have done this by arbitrarily defining an ‘extra smoothing region’ around any hole, and performing twice as many smooths in this region as in the rest of the domain. One can imagine more sophisticated schemes, which look at derivatives of the solution or the local truncation error as indicators of where the extra smoothing should be performed and how much extra work should be performed there.

3. It may be the case that pre-CGC smoothing is much more effective than post-CGC smoothing for a given problem, particularly if only one V-cycle is performed. In such cases concentrating the bulk of the smoothing operations into the pre-CGC smooths results in a faster route to the solution at a desired accuracy.

4. This repeats the advice of Alcubierre [38] (radial): Robin boundary conditions can be adequately mimicked by applying them only in the normal directions, thus simplifying the computer code and reducing the computation effort slightly. The Robin conditions should be applied at all grid levels; i.e. it is not the case that one should apply Robin conditions on the finest grid only and then use those values as Dirichlet conditions on coarser grids.

5. This tip is intended for use in situations where an exact solution is not available; we have less experience with these situations. However, we find that a naive quadratic extrapolation from nearby points is adequate to provide values for Dirichlet boundary conditions on the edge of the hole. Further (more technically), when monitoring the relative truncation error $\tau_{h}^{2h}$, points immediately adjacent to inner boundary points have erratic behaviour, and should not be considered in judging the behaviour of the solution.
We clearly have some further work ahead in order to consider more general systems in which our inner boundary data are not so easily obtained, and we also need to consider systems more complex than the Hamiltonian constraint for a conformally flat background, as treated in this paper. It is thus our hope that the techniques described here will also be of relevance for more interesting systems of elliptic equations. We are developing a solver for the full set of constraint equations (testing it using the Kerr–Schild-type binary black-hole data described in [39]), and see promising results using precisely the techniques given in this paper. Further improvements in the speed of multigrid scheme, such as the use of parallelism and adaptivity [40–42] will also likely be necessary for its practical application in a constrained evolution code.

The 2D and 3D codes described here are available for use by the community, by downloading from http://wwwrel.ph.utexas.edu/~shawley/mg_ex.html. We encourage other users of our approach. However, the codes are ‘as is’, and we cannot maintain them, nor correct problems that may arise from their use.

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References

[1] Arnowitt R, Deser S and Misner C W 1962 Gravitation: An Introduction to Current Research ed L Witten (New York: Wiley)
[2] York J W 1979 Sources of Gravitational Radiation ed L Smarr (Cambridge: Cambridge University Press)
[3] Siebel F and Hübner P 2001 Phys. Rev. D 64 024021
[4] Calabrese G, Pullin J, Sarbach O, Tiglio M and Reula O 2002 Preprint gr-qc/0209017
[5] Tiglio M 2003 Preprint gr-qc/0304062
[6] Yoneda G and Shinkai H 2003 Class. Quantum Grav. 20 L31
[7] Alcubierre M et al 2003 Preprint gr-qc/0305023
[8] Abrahams A A and Evans C R 1993 Phys. Rev. Lett. 70 2980
[9] Choptuik M W, Hirschmann E W, Liebling S L and Pretorius F 2003 Class. Quantum Grav. 20 1857
[10] Choptuik M W, Hirschmann E W, Liebling S L and Pretorius F 2003 Preprint gr-qc/0305003
[11] Schnetter E 2003 PhD Dissertation University of Tübingen in preparation
[12] Meier D L 2003 in preparation
[13] Anderson M and Matzner R A 2003 Preprint gr-qc/0307055
[14] Brandt A 1977 Math. Comput. 31 333
[15] Kidder L E and Finn L S 2000 Phys. Rev. D 62 084026
[16] Pfeiffer H P, Kidder L E, Scheel M A and Teukolsky S A 2003 Comput. Phys. Commun. 152 253
[17] Klasky S 1994 PhD Dissertation University of Texas at Austin
[18] Choptuik M W 2002 Personal communication
[19] Choquet-Bruhat Y, Isenberg J and York J W 2000 Phys. Rev. D 61 084034
[20] Dain S 2001, Phys. Rev. D 64 124002
[21] Maxwell D 2003 Preprint gr-qc/0307117
Multigrid methods on domains containing holes

[22] Brandt A 1982 Multigrid methods Lecture Notes in Mathematics vol 960, ed W Hackbusch and U Trottenburg (New York: Academic) pp 53–147

[23] Hackbusch W 1985 Multi-Grid Methods and Applications (Springer Series in Comp. Math. vol 4) (Berlin: Springer)

[24] Stüben K and Trottenburg U 1982 Multigrid Methods: Proceedings of Köln-Porz, 1981 ed W Hackbusch and U Trottenberg (Berlin: Springer)

[25] Wesseling P 1980 Numerical analysis Proc. (Dundee, 1979) (Lecture Notes in Mathematics vol 773) ed G A Watson (Berlin: Springer) p 164

[26] Wesseling P 1992 An Introduction to Multigrid Methods (Chilchester: Wiley) http://www.mgnet.org/mgnet-books-wesseling.html

[27] Briggs W L, Henson V E and McCormick S F 2000 A Multigrid Tutorial 2nd edn (Philadelphia: SIAM)

[28] Johansen H and Colella P 1998 J. Comput. Phys. 147 60

[29] Udaykumar H S, Mittal R, Rampunggoon P and Khanna A 2001 J. Comput. Phys. 174 345

[30] Brandt S and Brügmann B 1997 Phys. Rev. Lett. 78 3606

See also Brügmann B 1998 18th Texas Symp. on Relativistic Astrophysics and Cosmology (Chicago, 1996) ed A Olinto, J Frieman and D Schramm (Singapore: World Scientific)

[31] Press W H, Teukolsky S A, Vetterling W T and Flannery B P 2001 Numerical Recipes in Fortran 77 2nd ed (Cambridge: Cambridge University Press) p 862

[32] Choptuik M W 1999 Lecture Notes Taller de Verano 1999 de FENOMEC: numerical analysis with applications in theoretical physics

[33] Choptuik M W and Unruh W G 1986 Gen. Rel. Grav. 18 813

[34] Brandt A 1988 Class. Quantum Grav. 5 713

[35] Choptuik M W 1998 mgfas2d Lecture Notes for Physics 381C—Computational Physics (University of Texas at Austin) unpublished

[36] Pretorius F 2002 PhD Dissertation University of British Columbia pp 42–3

[37] York J W and Piran T 1982 Spacetime and Geometry ed R Matzner and L Shepley (Austin: University of Texas Press) p 145

[38] Alcubierre M 2003 Personal communication

[39] Bonning E, Marronetti P, Nielsen D and Matzner R A 2003 Phys. Rev. D 68 044019

[40] Griebel M and Zumbusch G 1998 Proc. ParCo ’97 ed E D’Hollander, G R Joubert, F J Peters and U Trottenberg (Amsterdam: Elsevier) pp 589–99

[41] Brown D and Lowe L 2003 Penn State Numerical Relativity Lunch Talk (21 Feb.) http://www.astro.psu.edu/~nrlunch/2003/2003-02-21_Brown/Transparencies.pdf

[42] Baker B 2002 PhD Dissertation University of Florida p 57