A remedy for constraint growth in Numerical Relativity

Gioel Calabrese

School of Mathematics, University of Southampton, Southampton, SO17 1BJ, UK

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Rapid growth of constraints is often observed in free evolutions of highly gravitating systems. To alleviate this problem we investigate the effect of adding spatial derivatives of the constraints to the right hand side of the evolution equations, and we look at how this affects the character of the system and the treatment of boundaries. We apply this technique to two formulations of Maxwell’s equations, the so-called fat Maxwell and the Knapp-Walker-Baumgarte systems, and obtain mixed hyperbolic-parabolic problems in which high frequency constraint violations are damped. Constraint-preserving boundary conditions amount to imposing Dirichlet boundary conditions on constraint variables, which translate into Neumann-like boundary conditions for the main variables. The success of the numerical tests presented in this work suggests that this remedy may bring benefits to fully nonlinear simulations of General Relativity.

I. INTRODUCTION

The $3+1$ decomposition of Einstein equations gives rise to a system of evolution equations and a set of constraints. Although it is true that, at the analytical level and in the absence of boundaries, if the constraints are satisfied on an initial spacelike hypersurface, they remain satisfied at later times by virtue of the evolution equations, this is not the case in numerical simulations. If the continuum initial data satisfy the constraints exactly, then they will only satisfy the discretized constraints up to truncation error. In many cases, initial errors grow exponentially, and sometimes even more rapidly. Whether the violent growth of the constraints is causing the crash of numerical codes, or is simply the effect of a more general growth in the error, is not altogether clear. However, the hope is that, if the constraint growth can be prevented or at least alleviated, the runtime of numerical simulations may increase.

In recent years a number of techniques have been proposed aimed at damping the constraints or, at least, controlling their growth. These are the $\lambda$-system [1], the fine-tuning of parameters multiplying the constraints that are added to the evolution equations [2], the dynamical adjustment of such parameters [3], and the addition of variational derivatives of a constraint energy to the evolution equations [4]. The method that we wish to investigate has remarkable similarities with the latter. When time-like boundaries are present all of these methods require constraint-preserving boundary conditions to prevent the injection of constraint violations.

We begin with a simple observation. Consider the first order scalar equation on the real line,

$$u_t = iu_x,$$  \hspace{1cm} (1)

where $i^2 = -1$, supplemented with smooth initial data. If we make the ansatz $u(t,x) = e^{i\omega x} \hat{u}(t,\omega)$, $\omega \in \mathbb{R}$, and substitute it into (1), we obtain $\hat{u}_t = -\omega \hat{u}$. The fact that the solution, $u(t,x) = e^{i\omega x - \omega t} \hat{u}(0,\omega)$, allows for unbounded growth [20] shows that the initial value problem is ill-posed and, therefore, cannot be consistently discretized in a stable way. Now we modify our problem and assume that the constraint

$$C \equiv u_x + iu = 0$$  \hspace{1cm} (2)

has to hold. Clearly, if $u$ satisfies Eq. (1), then $C_t = iC_x$, i.e., the constraint propagation problem is also ill-posed. A crucial point is that we are allowed to add constraints and/or derivatives of constraints to the right hand side of the evolution equations without affecting the space of physical solutions (i.e., solutions that satisfy the constraints). For example, adding a spatial derivative of the constraint to the right hand side of Eq. (1) leads to

$$u_t = iu_x + C_x = 2iu_x + u_{xx}. \hspace{1cm} (3)$$

This equation is parabolic and, most importantly, gives rise to a well-posed initial value problem for both the main and the constraint propagation systems. Not only does the problem no longer suffer from unbounded growth of the constraints, but the modification also damps the high frequency constraint violations. Furthermore, in the presence of boundaries, we can impose homogeneous Dirichlet boundary conditions on the constraint, $C = 0$, which, when translated in terms of the main variables become of Neumann type, $u_x = -iu$. This example, although trivial, clearly illustrates the potential benefits of dissipation. It allowed us to convert an ill-posed initial value problem into a well-posed initial-boundary value problem [21].

In this paper we investigate the effect of adding spatial derivatives of the constraints to the evolution equations for two formulations of Maxwell’s equations, the so-called fat Maxwell [5] (first order) and the Knapp-Walker-Baumgarte (KWB) [6] (first order in time, second in space) systems. As expected, the modification destroys the hyperbolic character of the systems. However, if done carefully, it can lead to mixed hyperbolic-parabolic systems both for the evolution equations and the evolution of the constraints, such that the high frequency components of the constraints are damped.

In the presence of timelike boundaries the systems that we analyze are such that constraint-preserving boundary
conditions amount to imposing homogeneous Dirichlet boundary data on the constraints, which translate into Neumann-like boundary conditions for the main system. Compared to standard constraint-preserving boundary conditions for hyperbolic problems, those that we obtain can be much simpler and possibly more robust. For example, if the constraint propagation system is strongly parabolic, then at the boundary we can impose that all constraints vanish, which is less involved than computing the incoming characteristic constraints and, as usually done, trading the normal with time and tangential derivatives using the evolution equations. Further, the modified problems allow for a greater number of constraint components to be set to zero. Unfortunately, — and this is presumably the most regrettable feature of this technique — due to the loss of finite speed of propagation, the time step needs to be proportional to the square of the mesh spacing in order to achieve numerical stability (and convergence) with explicit finite difference schemes.

Parabolic systems have received little attention in numerical relativity with some notable exceptions, in which the aim was primarily to promote elliptic gauge conditions to parabolic equations. Although the technique of adding spatial derivatives of the constraints has been previously employed by Yoneda and Shinkai and by Fiske, the analysis of the character and the study of appropriate boundary conditions for the modified systems, to our knowledge, is new.

We recall some basic definitions that will be used throughout the paper. Consider the systems of partial differential equations in one space dimension

\[ \partial_t u = A \partial_x^2 u + B \partial_x u + Cu, \]
\[ \partial_t v = D \partial_x v + Ev, \]

where \( A, B, C, D, \) and \( E \) are constant square matrices. System \( 1 \) is said to be strongly parabolic if the eigenvalues of \( A + A^T \) are positive. We call system \( 4 \) symmetric hyperbolic if \( D = D^T \). In the presence of boundaries and with appropriate initial and boundary conditions both systems admit a well-posed initial-boundary value problem as does the coupled mixed hyperbolic-parabolic system

\[ \partial_t \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} A \partial_x^2 + B \partial_x + C F \partial_x + G \\ L \partial_x + M D \partial_x + E \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}, \]

for any choice of the coupling matrices \( F, G, L, \) and \( M \). Notice that the character of system \( 6 \) is entirely determined by the two matrices \( A \) and \( D \).

The paper is organized as follows. In Sec. \( 11 \) we introduce the fat Maxwell system, appropriately add spatial derivatives of constraints and analyze the resulting initial-boundary value problem. A similar analysis is then repeated for the KWB system in Sec. \( 11 \). In Sec. \( 11 \) after describing the discretization of the system and, particularly, of the boundary conditions, we summarize the results of our numerical experiments. We conclude with some final remarks in Sec. \( 14 \). In appendix \( 1 \) we discuss an energy conserving discretization for the wave equation in second order form, allowing for Sommerfeld boundary conditions. This discretization is used for the hyperbolic sector of the KWB system.

We use units where \( c = \mu_0 = \epsilon_0 = 1 \) and adopt the Einstein summation convention.

II. THE FAT MAXWELL SYSTEM

The vacuum Maxwell equations on a Minkowski background in Cartesian coordinates are given by

\[ \partial_t E_i = \epsilon_{ijk} \partial^j B^k, \]
\[ \partial_t B_k = -\epsilon_{ijk} \partial^j E^k, \]
\[ \partial^k E_k = 0, \]
\[ \partial^k B_k = 0. \]

In terms of the potentials, \( \phi \) and \( A_i \), the electric and magnetic fields are

\[ E_i = -\partial_t A_i - \partial_i \phi, \]
\[ B_i = \epsilon_{ijk} \partial^j A^k. \]

If we introduce the variables \( D_{ij} = \partial_i A_j \), we can rewrite Maxwell’s equations in the form

\[ \partial_t E_i = \partial^k (D_{ik} - D_{ki}), \]
\[ \partial_t D_{ij} = -\partial_i E_j - \partial_j \partial_i \phi, \]
\[ C \equiv \partial^k E_k = 0, \]
\[ C_{ijk} \equiv \partial_i D_{jk} - \partial_j D_{ik} = 0, \]

where we used the identity \( \epsilon_{ijk} \epsilon^{ilm} = \delta^l_j \delta^m_k - \delta^m_j \delta^l_k \). This system has 12 variables that depend on the space-time coordinates and is subject to 10 constraints. One can readily verify that the constraints propagate trivially,

\[ \partial_t C = 0, \]
\[ \partial_t C_{ijk} = 0, \]

and that the evolution system is weakly hyperbolic, i.e., it cannot be diagonalized. However, by appropriately adding constraints to the right hand side of the evolution equations

\[ \partial_t E_i = \partial^k (D_{ik} - D_{ki}) + C_{ikk}, \]
\[ \partial_t D_{ij} = -\partial_i E_j - \partial_j \partial_i \phi + \delta_{ij} C, \]

one can ensure that both the main evolution system and the evolution of the constraint variables are symmetric hyperbolic. We note that this modification corresponds to setting \( \gamma_1 = 2 \) and \( \gamma_2 = 1 \) in the two parameter family of formulations of Lindblom et al. \( 5 \).
Any first order, linear, homogeneous, constant coefficient, symmetric hyperbolic system with no lower order terms admits, by definition, a conserved energy. An energy, in this context, is an integral over the spatial domain, $\Omega$, of a positive definite quadratic form of the main variables. The energies
\[
E = \frac{1}{2} \int_{\Omega} \left( E^i E_i + D^{ij} D_{ij} \right) \, d^3 x ,
\]
\[
E_C = \frac{1}{2} \int_{\Omega} \left( C^2 + \frac{1}{2} C^{ij} C_{ij} \right) \, d^3 x ,
\]
for example, are conserved up to contributions due to the boundary (the conservation of $E$ requires the Coulomb gauge, $\phi = 0$, which will henceforth be assumed). An immediate consequence of this is that, if $\Omega = \mathbb{R}^3$ or $\Omega = T^3$, the energy associated with an initial violation of the constraints will be preserved during evolution. We now show that by adding spatial derivatives of the constraints to the evolution equations it is possible to improve on this.

The general idea is to add constraints and/or derivatives of constraints to the right hand side of the evolution equations that generate decaying or damping terms in the constraint propagation system. Consider the following modification of the main evolution system
\[
\partial_t E_i = \ldots + \mu \partial_t C ,
\]
\[
\partial_t D_{ij} = \ldots + \mu \partial_t C_{ij} ,
\]
The evolution of the constraint variables becomes
\[
\partial_t C = \partial^i C_{ikk} + \mu \partial^i \partial_t C ,
\]
\[
\partial_t C_{ijk} = 2 \partial^i \delta_{ijk} C + 2 \mu \partial^i \partial^j C_{ij} \partial_t C_{ijk} .
\]

By following this procedure, we have lost symmetric hyperbolicity. It is essential to check whether the modified systems still admit a well-posed initial value problem. We start by showing that both systems, (13)–(14) and (15)–(16), satisfy a necessary condition for well-posedness, the Petrovskii condition (14). We will show that for positive values of the parameter $\mu$ most Fourier components of the constraint variables are damped. We then give an energy estimate for the evolution of the constraints systems and, as a byproduct, obtain constraint-preserving boundary conditions. Our attempts at deriving an estimate for the main system have not been successful when boundary conditions consistent with the constraints are imposed. Nevertheless, we found the one dimensional reduction of the problem to be well-posed and therefore used it as a tool for obtaining appropriate boundary conditions for the main system. The rationale being that any boundary condition that makes the reduced problem ill-posed would be unsuitable in higher dimensions.

Let $u_t = P(\partial_x)u$ be a system of linear constant coefficient partial differential equations in $d$ dimensions. Assume for the moment that there are no boundaries. According to the Petrovskii condition, it must be possible to bound the real parts of the eigenvalues of the symbol, or Fourier transform, of the differential operator, $P(i\omega)$, by a real constant $\alpha$, which is independent of $\omega$. For scalar equations this condition is also sufficient.

To compute the symbols of (13)–(14) and (15)–(16) we use the substitution $\partial_k \rightarrow i\omega_k = i|\omega|\hat{\omega}_k$, where $\hat{\omega}_k \hat{\omega}_k = 1$. From the evolution equations we get
\[
\partial_t E_\omega = i|\omega|D_{AA} - \mu \omega^2 E_\omega ,
\]
\[
\partial_t D_{AA} = -i|\omega|E_\omega ,
\]
\[
\partial_t D_{AB} = 2i|\omega|E_\omega - \mu \omega^2 D_{AB} ,
\]
\[
\partial_t C_{AB} = \partial^\mu D_{AB} E_\omega ,
\]
where $u_\omega = \hat{\omega}_k u_k$, $u_\omega = \hat{\omega}_k u_k$, $\hat{A}_k \hat{B}_k = \delta_{AB}$, $\hat{\omega}_k \hat{A}_k = 0$, and $u_{AB} = u_{AB} - \frac{1}{2} \delta_{AB} u_{CC}$. The evolution of the constraints yields
\[
\partial_t C = i|\omega|C_{AA} - \mu \omega^2 C ,
\]
\[
\partial_t C_{AA} = 2i|\omega|C - \mu \omega^2 C_{AA} ,
\]
\[
\partial_t C_{AB} = -\mu \omega^2 C_{AB} ,
\]
\[
\partial_t C_{AB} = -\mu \omega^2 C_{AB} ,
\]
\[
\partial_t C_{AB} = 0 .
\]

The eigenvalues of the Fourier transformed systems form a subset of
\[
\{ \pm |\omega|, -\mu \omega^2 \pm i \sqrt{2|\omega|}, -\mu \omega^2, 0 \} .
\]

Hence the Petrovskii condition is satisfied provided that $\mu \geq 0$. In particular, this shows that for $\mu > 0$ the high frequency components of most constraints are rapidly damped.

We now calculate the time derivative of (12). This is given by
\[
\frac{d}{dt} E_C = \int_\Omega \left( C C_{n,AA} + \mu C \partial_n C + \mu C_{n,AK} \partial_l C^{l,Ak} \right) \, d^3 S
\]
\[
- \mu \int_\Omega \left( \partial^i C \partial_t C + \partial_t C^{ij} \partial^i C_{ij} \right) \, dx .
\]

Clearly, the volume integral gives a non-positive contribution to the time derivative of the energy and, therefore, by controlling the boundary term one can ensure that the energy associated with the constraints is non-increasing. Boundary conditions that can be used for this purpose are
\[
C = 0 , \quad C_{n,AK} = 0 .
\]

When these 7 conditions are enforced we obtain the inequality
\[
\frac{d}{dt} E_C = -\mu \int_\Omega \left( \partial^i C \partial_t C + \partial_t C^{ij} \partial^i C_{ij} \right) \, d^3 x \leq 0 .
\]
where specifiable boundary data and imply maximally dissipative boundary conditions to the 5 Neumann-like boundary conditions. We are free to specify

the parabolic sector require a boundary condition and comparing with Eq. (6). The 7 variables belong-

the quarter space problem. We assume that the bound-

in the presence of boundaries we were not able to obtain an energy estimate using conditions \( \mathbb{E} \). We therefore look at simple necessary conditions for well-posedness for the quarter space problem. We assume that the boundary is located at \( x = 0 \) and that \( \Omega = \{(x, y, z) \in \mathbb{R}^3 | x \geq 0 \} \). If the variables depend only on \( x \) and \( t \), the system becomes

\[
\begin{align*}
\partial_t E_1 &= +\partial_x D_{1A} + \mu \partial_x^2 E_1, \\
\partial_t E_A &= -\partial_x D_{1A}, \\
\partial_t D_{11} &= 0, \\
\partial_t D_{1A} &= -\partial_x E_A, \\
\partial_t D_{A1} &= -\partial_x D_{A1}, \\
\partial_t D_{AB} &= \delta_{AB} \partial_x E_1 + \mu \partial_x^2 D_{AB},
\end{align*}
\]

where \( A = 2, 3 \) and \( B = 2, 3 \). No matter what boundary conditions one uses for the main system, they should be such that the one dimensional reduction of the problem is well-posed. The equations above form a mixed hyperbolic-parabolic system. This can be seen by identifying \( u = \{E_1, D_{1k}\} \) and \( v = \{E_A, D_{1k}\} \), and comparing with Eq. \( \mathbb{E} \). The 7 variables belonging to the parabolic sector require a boundary condition each. Eq. \( \mathbb{E} \) provides us with the correct number of Neumann-like boundary conditions. We are free to specify maximally dissipative boundary conditions to the 5 variables of the hyperbolic sector,

\[
\begin{align*}
(w_{\text{in}} - S_{\text{AB}} w_{\text{out}}) |_{x=0} &= g_A, 
\end{align*}
\]

where \( S \) is a sufficiently small \( 2 \times 2 \) matrix, \( g_A \) is freely specifiable boundary data and

\[
\begin{align*}
w_{\text{in}} &= \frac{1}{\sqrt{2}}(E_A + D_{1A}), \\
w_{\text{out}} &= \frac{1}{\sqrt{2}}(E_A - D_{1A}),
\end{align*}
\]

are the ingoing and outgoing characteristic variables. This gives a total of 9 boundary conditions for the main evolution system, 7 of which ensure constraint preservation \( \mathbb{E} \).

A description of the discretization of the initial-boundary value problem and the results of the numerical experiments are given in Sec. \( \mathbb{E} \).

### III. THE KWB SYSTEM

In Ref. \( \mathbb{E} \) Knapp, Walker, and Baumgarte, introduced a formulation of Maxwell’s equations which shares some features with the Baumgarte-Shapiro-Shibata-Nakamura formulation of Einstein equations \( \mathbb{E} \). In vacuum and on a Minkowski background in Cartesian coordinates the equations take the form

\[
\begin{align*}
\partial_t A_i &= -E_i - \partial_t \phi, \\
\partial_t E_i &= -\partial_t \partial^j A_j + \partial_t \Gamma, \\
\partial_t \Gamma &= -\partial_j \partial^j \phi.
\end{align*}
\]

where the fields \( A_i, E_i \) and \( \Gamma \) are subject to the constraints

\[
\begin{align*}
C_E &\equiv \partial^j E_j = 0, \quad (23) \\
C_\Gamma &\equiv \partial_t A^j - \Gamma = 0. \quad (24)
\end{align*}
\]

The system contains second spatial derivatives and is symmetric hyperbolic \( \mathbb{E} \). As the authors of \( \mathbb{E} \) pointed out, in this system the constraints propagate according to the wave equation

\[
\begin{align*}
\partial_t C_E &= -\partial_j \partial^j C_\Gamma, \\
\partial_t C_\Gamma &= -C_E, \\
\end{align*}
\]

which is to be contrasted with the static constraint evolution of the original Maxwell system, Eqs. \( \mathbb{E} \).

The constraint system \( \mathbb{E}, \mathbb{E} \) conserves the following energy

\[
E_C = \frac{1}{2} \int_{\Omega} (C_E^2 + \partial^j C_j \partial_t C_\Gamma) d^3 x. \quad (27)
\]

If one sets \( \phi = 0 \) and modifies the evolution equations according to

\[
\begin{align*}
\partial_t A_i &= \ldots + \mu \partial_t C_\Gamma, \\
\partial_t E_i &= \ldots + \mu \partial_t C_E, \\
\partial_t \Gamma &= \lambda C_\Gamma = \lambda \partial_t A^2 - \Gamma, \\
\end{align*}
\]

which can be identified with Eqs. (22)–(23) of Fiske \( \mathbb{E} \), the evolution of the constraints becomes

\[
\begin{align*}
\partial_t C_E &= -\partial^j \partial_j C_\Gamma + \mu \partial^j \partial_t C_E, \\
\partial_t C_\Gamma &= -C_E + \mu \partial^j \partial_t C_\Gamma - \lambda C_\Gamma. \\
\end{align*}
\]

The evolution equations were modified so that \( \mathbb{E} \) and \( \mathbb{E} \) would acquire damping and friction terms.

Rather than estimating the energy \( \mathbb{E} \) we observe that, if \( \mu > 1/2 \), the constraint propagation system is strongly parabolic and an energy estimate for the constraint system can be obtained directly in \( L_2 \). The time derivative of

\[
E_C = \frac{1}{2} \int_{\Omega} (C_E^2 + C_\Gamma^2) d^3 x
\]

is

\[
\frac{d}{dt} E_C = \int_{\partial \Omega} (-C_E \partial_n C_\Gamma + \mu C_E \partial_n C_E + C_\Gamma \partial_n C_\Gamma) d^2 S + \int_{\Omega} (\partial^i C_E \partial_i C_\Gamma - \mu \partial^i C_E \partial_i C_E - \mu \partial^i C_\Gamma \partial_i C_\Gamma) d^3 x + \int_{\Omega} (-C_\Gamma C_E - \lambda C_\Gamma^2) d^3 x. \quad (34)
\]

The use of Dirichlet boundary conditions,

\[
C_E = C_\Gamma = 0, \quad (35)
\]
ensures that the boundary term of Eq. 34 vanishes. Furthermore, the volume term containing spatial derivatives is non-positive. Thus, an energy estimate can be obtained [24].

We now place a boundary at $x = 0$ so that $\Omega = \{(x, y, z) \in \mathbb{R}^3 | x \geq 0\}$. By ignoring any $y$ and $z$ dependence the hyperbolic-parabolic character of the system becomes evident (the introduction of the auxiliary variable $W_B = \partial_x A_B$ may be helpful for this analysis)

$$\begin{align*}
\partial_t A_1 &= -E_1 + \mu \partial_x^2 A_1 - \mu \partial_x \Gamma, \\
\partial_t A_B &= -E_B, \\
\partial_t E_1 &= -\partial_x^2 A_1 + \partial_x \Gamma + \mu \partial_x^2 E_1, \\
\partial_t E_B &= -\partial_x^2 A_B, \\
\partial_t \Gamma &= \lambda \partial_x A_1 - \lambda \Gamma.
\end{align*}$$

For $\mu > 1/2$ we can identify a parabolic sector $\{A_1, E_1\}$ and a hyperbolic sector $\{A_B, E_B, \Gamma\}$. Dirichlet boundary conditions on the constraints, $C_E = 0$, $C_\Gamma = 0$, correspond to Neumann-like boundary conditions on the main variables of the parabolic sector. Maximally dissipative boundary conditions can be imposed on the variables of the hyperbolic sector,

$$(\partial_x A_B + E_B)|_{x=0} = 0. \tag{36}$$

Numerical experiments with the modified KWB system indicate that the discrete approximation of the initial-boundary value problem is stable. More details are given in the next Section. In Appendix A we analyze the accuracy and stability of discretized maximally dissipative boundary conditions, such as Eq. (36), for the one dimensional wave equation in second order form.

IV. NUMERICAL IMPLEMENTATION

To discretize our problems we use the method of lines, whereby space is discretized while time is left continuous. We then integrate the resulting system of ordinary differential equations using 4th order Runge-Kutta. We take our domain to be $\Omega = [0, 1]^3$ and use periodic boundary conditions in $y$ and assume no dependence on $z$. We introduce a grid such that the points $(0, j, k)$ belong to the boundary, $x = 0$. In the interior we approximate the first spatial derivatives with centered differencing operators and the second spatial derivatives according to

$$\partial_x \partial_x u \rightarrow \begin{cases} 
D_{+,m} D_{+,m-1} u_{ijk} & l = m \\
D_{0,m} D_{0,m-1} u_{ijk} & l \neq m
\end{cases}$$

where $hD_{+,j} = u_{j+1} - u_j$, $hD_{-,j} = u_j - u_{j-1}$, and $2D_0 = D_+ + D_-$. Thus, the discretization in the interior is second order accurate.

The discretization of the boundary conditions is based on algorithms for which convergence proofs are available, at least for simple toy model problems [13]. For example, one can show that for the one-way advective equation, $u_t = u_x$, $x \geq 0$, one can use one-sided differencing at the boundary, $\frac{\partial u}{\partial x} |_{x=0} = D_x u_0$. For the heat equation, $u_t = u_{xx}$, $x \geq 0$, with Neumann boundary condition $u_x(t, 0) = 0$, one can use the approximation $D_0 u_0(t) = 0$ which, when combined with the evolution equation at $i = 0$ becomes $\frac{du}{dt} = 2D_x u_0$. Both cases give global second order convergence.

To simplify the numerical implementation of the boundary conditions we found it convenient to introduce a ghost zone consisting of an extra grid point, $i = -1$, to the left of the boundary, so that derivatives could be computed at $i = 0$ as if it were an interior point. In the fat Maxwell case we use the following prescription to populate the ghost zone: we use the Neumann-like boundary conditions [13] and use second order extrapolation for the remaining fields, $\{E_A, D_{1A}\}$. Explicitly,

$$\begin{align*}
0 &= D_{0x} E_{1,0,jk} + D_{xy} E_{2,0,jk} + D_{0z} E_{3,0,jk}, \\
0 &= D_{0x} D_{A,m,0,jk} - \Gamma_{A,m,0,jk}, \\
0 &= D_{+x} D_{-x} E_{A,0,jk}, \\
0 &= D_{+x} D_{-x} D_{1m,0,jk}.
\end{align*}$$

Note that when combined with a second order centered difference at $i = 0$, second order extrapolation is equivalent to first order one-sided differencing. Eq. 19 with $S_{IB} = g_A = 0$ is then used to prescribe the incoming fields of the hyperbolic part. The new variables are computed by solving the system

$$\begin{align*}
E_A^{(\text{new})} + D_{1A}^{(\text{new})} &= 0, \\
E_A^{(\text{new})} - D_{1A}^{(\text{new})} &= E_A^{(\text{old})} - D_{1A}^{(\text{old})}
\end{align*}$$

In the KWB case the boundary treatment is slightly different due to the hyperbolic role that some second spatial derivatives play in the evolution equations. The theory of difference approximations for second order hyperbolic systems is much less developed than the correspondent one for first order systems (for some recent developments see Ref. 13). Based on the energy method for semi-discrete systems, in Appendix A we give a proof of second order convergence for a particular discretization of the one dimensional wave equation, $u_{tt} = u_{xx}$, $x \geq 0$, with Sommerfeld boundary conditions, $u_{tt}(t, 0) = u_x(t, 0)$. This result is used in the discretization of boundary condition 36.

As in the fat Maxwell case, we introduce a ghost zone and populate it using the following equations

$$\begin{align*}
0 &= D_{0x} A_{1,0,jk} + D_{xy} A_{2,0,jk} + D_{0z} A_{3,0,jk} - \Gamma_{0,jk}, \\
0 &= D_{0x} A_{B,0,jk} + E_{0,jk}, \\
0 &= D_{0x} E_{1,0,jk} + D_{xy} E_{2,0,jk} + D_{0z} E_{3,0,jk}, \\
0 &= D_{+x} D_{-x} E_{B,0,jk}, \\
0 &= D_{+x} D_{-x} \Gamma_{0,jk}.
\end{align*}$$

The first and third conditions correspond to the vanishing of the constraints, Eq. 35. The second condition is the discretization of Eq. 36 done according to the
choose larger time steps. In the KWB case, instead, we must constraints. We opt for $\mu > 1$ could use $C/E$ something reasonably small, 1.

tem there is no restriction on the value of $\mu k/h^2$.

Fig. 1, we test our schemes with constraint violating ini-

tial data corresponding to a sufficiently smooth pulse of

an oblique direction with respect to the boundary. For the

fat Maxwell system it is obtained from the potentials $\phi = 0$

and $A = \frac{1}{h} \sin(\pi (x + 2y + \sqrt{5}t))(0, 0, 1)$, while for the KWB

system from $\phi = 0$ and $A = \frac{1}{h} \sin(\pi (x + 2y + \sqrt{5}t))(2, -1, 0)$.

In the fat Maxwell case the time step, $k$, is chosen so that

$4\mu k/h^2 = 1$, where $h$ is the spatial mesh spacing, and we set

$\mu = 1/10$. In the KWB case we used $2\mu k/h^2 = 1$, $\mu = 1$ and $\lambda = 10$.

Values of $Q$ close to 2 indicate second order convergence for the main variables.

Fig. 2: We plot the value of $E_{C,2}^{1/2}$, Eqs. (A2) and (A4), for the fat Maxwell system (top) and the KWB system (bottom) for three different resolutions. The curves are labeled according to the number of grid points used in each spatial direction. We give constraint violating initial data consisting of a sufficiently smooth pulse of compact support to all fields. In both cases the domain is $\Omega = [0, 1]^2$, having dropped the dependence in the $x$ direction, and we impose periodic boundary conditions in the $y$ direction. At $x = 0$ and $x = 1$ we use the boundary conditions outlined in Sec. IV. The values of the parameters and the size of the time step $k$ are chosen as in Fig. 1. The noise in the curves of the KWB case are likely due to the fact that the energy being monitored, Eq. (27), contains spatial derivatives which are discretized using $D_0$ operators.

V. CONCLUDING REMARKS

In this work we investigated the effect of adding spatial derivatives of constraints to the main evolution system. We studied the initial-boundary value problem for two different formulations of Maxwell’s equations, the fat Maxwell system and the Knapp-Walker-Baumgarte formulation. We noticed that the modification alters the character of the systems, transforming them into mixed hyperbolic-parabolic problems. Parabolicity introduces two remarkable effects. First, it damps the high fre-
FIG. 3: At a fixed resolution of \( h = 1/50 \) and with periodic boundary conditions and no dependence in \( z \) we compare the decay of the constraint energies, Eqs. (12) and (27), between the modified and unmodified systems for the fat Maxwell (top) and the KWB (bottom) systems. As in Fig. 2, the initial data is a constraint violating pulse of compact support to all fields. Although this cannot be seen from the plots, at time \( t = 0 \) the constraint energy of the modified and unmodified systems coincide.

frequency components of constraint violations (whereas in the KWB case the damping affects all constraints, in the fat Maxwell system some constraints are not damped). Second, it allows for Dirichlet boundary conditions for the constraints which naturally translate into Neumann-like boundary conditions for the main system. These boundary conditions are constraint-preserving and, if the evolution of the constraints can be made strongly parabolic, their expression is simpler than that of the original hyperbolic system. Furthermore, whereas other techniques, such as the \( \lambda \)-system \([1]\), require a substantial enlargement of the main system, this method leaves the number of variables unchanged. Although we were unsuccessful in obtaining an energy estimate for the main evolution systems, our numerical tests not only confirmed that the constraints are damped, but also indicated that the discretized systems are stable.

The stringent requirement on the time step \( k \) is possibly the greatest drawback of this technique. Whereas for hyperbolic problems \( k \) typically has to be proportional to the mesh spacing, \( h \), in parabolic or mixed hyperbolic-parabolic problems it has to be proportional to \( h^2 \). To circumvent this restriction one could use implicit or semi-implicit schemes. However, we have not yet experimented with such schemes.

The damping terms introduced by the spatial derivatives of constraints vanish on physical (constraint satisfying) solutions. This indicates that dissipation will not detrimentally affect such solutions and, although constraint violations can travel at an infinite speed, any constraint satisfying solution will propagate information at a finite speed. Of course, at the numerical level, the numerical speed of propagation usually only coincides with the continuum one up to truncation errors and it is even possible for high frequency modes to travel in the wrong direction \([14]\).

It is important to realize that in the nonlinear or variable coefficient case, extra care is required for the successful application of this technique. The coefficients in front of the parabolic terms should never become negative, as this would immediately allow for unbounded growth and lead to instabilities. Artificial dissipation of the Kreiss-Oliger type should still be added to the right hand side in order to damp high frequency components of the hyperbolic sector. In addition, this technique, just like most of the available cures for constraint growth, cannot be expected to cure instabilities, such as “gauge instabilities”, that are not constraint violating.

The technique illustrated in this work requires a different treatment of the excision boundaries, often used in numerical simulations of spacetimes containing black holes. Whereas in hyperbolic formulations no boundary conditions are needed at the excision surface, provided that this is purely outflow, parabolicity demands boundary conditions. Our expectation is that the use of Dirichlet boundary conditions for the constraints at the excision boundary will help to prevent the growth of constraints near this troublesome region.

In this work we stressed how parabolicity can be obtained by adding spatial derivatives of constraints to the evolution equations. For systems, such as the ones studied in this paper, that have first order constraints, this is the only way it can be achieved. However, for systems containing constraints with second spatial derivatives (like the Hamiltonian constraint of General Relativity) one may obtain parabolicity by appropriately adding such constraints without further differentiation. This approach of adding constraints and/or spatial derivatives of constraints to the evolution equations could be pushed further and one could consider the possibility of adding higher order spatial derivatives of constraints. However, in general, adding second spatial derivatives of first order constraints or first spatial derivatives of second order constraints will not damp high frequency components. It
will only render the constraint propagation more disper-
sive. On the other hand, adding third spatial derivatives 
of first order constraints or second spatial derivatives of 
second order constraints can help to dissipate the high 
frequencies. Certainly, it is preferable to avoid increasing 
the order of the formulation, as this would complicate 
the treatment of boundaries.

Although the problems to which our technique was ap-
plied do not present the full range of difficulties contained 
in Einstein’s equations, based on the success of the tests 
that we presented we hope that the technique may prove 
helpful in a more complex situation. Its effectiveness in 
non-linear problems of General Relativity will be assessed 
in future works.

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APPENDIX A: A DISCRETIZATION OF THE 
SECOND ORDER WAVE EQUATION WITH 
SOMMERFELD BOUNDARY CONDITIONS

Consider the wave equation,
\[ \partial_t^2 \phi(t, x) = \partial_x^2 \phi(t, x) , \quad (A1) \]
on the real line with appropriate initial data,
\[ \phi(0, x) = f^{(1)}(x) , \quad (A2) \]
\[ \partial_t \phi(0, x) = f^{(2)}(x) . \quad (A3) \]
The analysis that follows can be readily applied to the 
first order in time and second order in space formulation
\[ \partial_t \phi = T , \]
\[ \partial_t T = \partial_x^2 \phi . \]

As an immediate consequence of integration by parts we 
have that the energy \( E = \int \left( (\partial_t \phi)^2 + (\partial_x \phi)^2 \right) dx \) is conserved by any solution of the wave equation. If we dis-
cretize the second space derivative with the second or-

\begin{align*}
\frac{d^2 \phi_j}{dt^2} &= D_+ D_- \phi_j , \\
\frac{d^2 \phi_0}{dt^2} &= 2 \left( D_+ \phi_0 - \frac{d \phi_0}{dt} \right) / h ,
\end{align*}

which uses centered instead of one-sided differencing is 
not a conserved quantity, unless the right hand side of 
Eq. (A7) is replaced by \( D_0^2 \phi_j \). However, this would re-
quire a larger stencil and would not dissipate the highest 
frequency mode, \( \phi_j = (-1)^j \).

We now introduce an artificial boundary at \( x = 0 \) and 
take our domain to be \( x \geq 0 \). We are interested in finding 
approximations for the homogeneous Sommerfeld bound-
ary condition
\[ \phi(t, 0) = \phi_x(t, 0) , \quad (A6) \]

which lead to a second order accurate scheme. The initial 
data are assumed to be compatible with the boundary 
condition, i.e.,
\[ \frac{\partial^n}{\partial x^n} \left( f^{(2)}(x) - \partial_x f^{(1)}(x) \right) \bigg|_{x=0} = 0 . \]

Consider the approximation
\[ \frac{d \phi_0}{dt} = D_0 \phi_0 . \quad (A7) \]
This requires the introduction of \( \phi_{-1} \). However, by com-
bining (A7) with the evolution equation at \( j = 0 \),
\[ \frac{d \phi_0}{dt} = D_+ D_- \phi_0 , \]
we can eliminate \( \phi_{-1} \) from the semi-discrete system. We 
observe that the one-sided finite difference operators \( D_{\pm} \) satisfy the summation by parts rule
\[ (u, D_{\pm} v)_{-\infty, +\infty} = - (D_{\mp} u, v)_{-\infty, +\infty} , \]

where
\[ (u, v)_{r,s} = \sum_{j=r}^s u_j v_j h , \]
it follows that any solution of (A3) conserves the discrete 
energy
\[ E = \left( \frac{d \phi}{dt}, \frac{d \phi}{dt} \right)_{-\infty, +\infty} + (D_+ \phi, D_- \phi)_{-\infty, +\infty} . \quad (A5) \]

Note that the similar expression
\[ E_0 = \left( \frac{d \phi}{dt}, \frac{d \phi}{dt} \right)_{-\infty, +\infty} + (D_0 \phi, D_0 \phi)_{-\infty, +\infty} \]
where
\[ \frac{d \phi_j}{dt} = D_+ D_- \phi_j , \quad j = 1, 2, 3, \ldots , \quad (A8) \]
\[ \frac{d^2 \phi_0}{dt^2} = 2 \left( D_+ \phi_0 - \frac{d \phi_0}{dt} \right) / h , \quad (A9) \]

with initial data
\[ \phi_j(0) = f^{(1)}(x_j) , \quad (A10) \]
\[ \frac{d \phi_j}{dt}(0) = f^{(2)}(x_j) . \quad (A11) \]

We conclude this appendix by proving that the semi-discrete approximation (A8)–(A11) of the initial-
boundary value problem (A1)–(A3) and (A6) is stable 
and second order convergent.
We denote by \( \phi_c(t, x) \) the solution of the continuum problem \( A^{11} \) and \( \phi^i(t) \) the grid function satisfying the semi-discrete approximation \( A^{10} \). The norm with respect to which we wish to prove stability and convergence is the one associated with the scalar product

\[
2(u, v)_h = \frac{1}{2} \frac{d u_0}{d t} \frac{d v_0}{d t} h + \left( \frac{d u}{d t}, \frac{d v}{d t} \right)_{1, +\infty} + (D_+ u, D_+ v)_{0, +\infty}.
\]

The fact that the time derivative of \( \phi \) divided that higher derivatives of the exact solution are appropriately bounded, we can estimate the norm of the error,

\[
\frac{d}{dt} \| w \|^2_h = \frac{1}{2} \frac{d w_0}{d t} \frac{d^2 w_0}{d t^2} h + \left( \frac{d w}{d t}, \frac{d^2 w}{d t^2} \right)_{1, +\infty}
+ (D_+ w, D_+ \frac{d w}{d t})_{0, +\infty}
= -\left( \frac{d w_0}{d t} \right)^2 + \frac{1}{2} \frac{d w_0}{d t} F_0 h + \left( \frac{d w}{d t}, F \right)_{1, +\infty}
\leq F_0^2 h^2 + \| w \|^2_h + \| F \|^2_{1, +\infty}.
\]

Integrating, we obtain the inequality

\[
\| w(t) \|^2_h \leq \int_0^t e^{t-\tau} F_0^2(\tau) h^2 d\tau + \int_0^t e^{t-\tau} \| F(\tau) \|^2_{1, +\infty} d\tau
= \mathcal{O}(h^4)
\]

showing that the scheme is second order convergent with respect to the norm induced by the scalar product \( A^{12} \).

It is interesting to note that the simpler approximation

\[
\frac{d^2 \phi_j}{d t^2} = D_+ D_- \phi_j, \quad j = 1, 2, 3, \ldots \quad (A13)
\]

although stable, reduces the global accuracy of the scheme to first order. A similar calculation to the one in the proof leads to the inequality

\[
\| w(t) \|^2_h \leq \mathcal{O}(h^2).
\]

[1] O. Brodbeck, S. Frittelli, P. Hübner, O. Reula, J. Math. Phys. 40, 909-923 (1999).
[2] M. Scheel, L. Kidder, L. Lindblom, H. Pfeiffer, and S. Teukolsky, Phys. Rev. D 66, 124005 (2002).
[3] M. Tiglio, gr-qc/0404027.
[4] D. Fiske, Phys. Rev. D 69, 047501 (2004).
[5] L. Lindblom, M. Scheel, L. Kidder, H. Pfeiffer, D. Shoemaker, and S. Teukolsky, gr-qc/0402075.
[6] A. Knapp, E. Walker, and T. Baumgarte, Phys. Rev. D 65, 064031 (2002).
[7] M. Iriondo and O. Reula, Phys. Rev. D 65, 044024 (2002).
[8] G. Calabrese, J. Lehner, and M. Tiglio, Phys. Rev. D 65, 104031 (2002).
[9] G. Calabrese, J. Pullin, O. Reula, O. Sarbach, and M. Tiglio, Commun. Math. Phys. 240, 373-395 (2003).
[10] B. Szilágyi and J. Winicour, Phys. Rev. D 68, 041501 (2003).
[11] J. Stewart, Class. Quantum Grav. 15, 2865 (1998).
[12] J. Balakrishna, G. Daus, E. Seidel, W. Suen, M. Tobias, E. Wang, Class. Quantum Grav. 13 L135-L142 (1996); M. Shibata, Phys. Rev. D 60, 104052 (1999); M. Shibata and K. Uryü, Phys. Rev. D 61, 064001 (2000); M. Alcubierre and B. Brügmann, Phys. Rev. D 63, 104006 (2001); K. Tod, Class. Quantum Grav. 8 L115 (1991); D. Garfinkle and J. Isenberg, math.dg/0306129.
[13] H. Shinkai and G. Yoneda, gr-qc/0209111.
[14] B. Gustafsson, H. Kreiss, and J. Oliger, Time dependent problems and difference methods (John Wiley & Sons, New York, 1995).
[15] M. Shibata and T. Nakamura, Phys. Rev. D 52, 5428 (1995).
[16] B. Baumgarte and S. Shapiro, Phys. Rev. D 59, 024007 (1999).
[17] C. Gundlach and J. Martin-Garcia, gr-qc/0402079.
[18] H. Kreiss, N. Petersson, and J. Yström, SIAM J. Numer. Anal. 40, 1940-1967 (2002); H. Kreiss, N. Petersson, and J. Yström, Difference approximations of the Neumann problem for the second order wave equation, UCRL-JC-153184. (2003).
[19] H. Kreiss and O. Ortiz, Lect. Notes Phys. 604, 359 (2002).
[20] By this we mean that it is not possible to find two constants \( K > 0, \alpha \geq 0, \) such that the bound \( \| u(t, \cdot) \| \leq \)
\( K e^{\alpha t} \| u(0, \cdot) \| \) holds for any smooth initial data.

[21] The addition of the term \(-iC\) to the right hand side of the evolution equation (1), would also have led to a well-posed initial-boundary value problem. However, this modification also gives rise to exponential growth of all Fourier components of the constraints.

[22] Notice that, in the absence of boundaries, if \( C = \text{const.} \) and \( \partial^i C_{ijk} = 0 \) then the energy associated with the constraints will remain constant.

[23] The fact that the 7 boundary conditions (18) allow for an energy estimate for the constraint propagation system and that any smaller number of conditions would make this problem ill-posed (for this purpose it is sufficient to look at its one dimensional reduction), demonstrates that 7 is the correct number of boundary conditions for system (15)–(16).

[24] To ensure that the volume term of Eq. (34) containing undifferentiated constraints is semidefinite negative, so that the inequality \( \frac{d}{dt} E_C \leq 0 \) holds, one could add the term \(-C_E\) to the right hand side of Eq. (30).