Toward Making the Constraint Hypersurface an Attractor in Free Evolution

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There is an abundance of empirical evidence in the numerical relativity literature that the form in which the Einstein evolution equations are written plays a significant role in the lifetime of numerical simulations. This paper attempts to present a consistent framework for modifying any system of evolution equations by adding terms that push the evolution toward the constraint hypersurface. The method is, in principle, applicable to any system of partial differential equations which can be divided into evolution equations and constraints, although it is only demonstrated here through an application to the Maxwell equations.

I. INTRODUCTION

The data analysis needs of the LIGO and LISA experiments have driven an interest in finding numerical solutions to the Einstein equations in astrophysically relevant situations. Wave forms from such numerical simulations can, once generated, be used as templates for finding gravitational wave signals in the experimental noise.

In order to find numerical solutions, however, one must make a 3+1 space-time split of the Einstein equations following some variation of the ADM formalism. When using free evolution techniques, which is the most common practice in numerical relativity today, a plethora of authors have found that the exact form of the evolution equations, in particular how the constraints are substituted into the evolution equations, plays a critical role in how stable the evolution will be (e.g. [2, 3, 4, 5, 6]). Although making such modifications to the evolution equations remains more of an art than a science, some authors have proposed well defined methods for making stability-friendly modifications.

Historically, Detweiler [7] seems to be one of the first authors to consider explicitly a method for adding terms proportional to the constraints to the evolution equations with the goal of improving simulation stability. He looked at the evolution of the constraints, and tried to add terms to the evolution equations of the fundamental variables that would drive the constraints to zero as the evolution progressed. This approach is very similar to the approach presented here.

Where the approach differs, however, is significant. Whereas Detweiler needed to add terms such that a negative-definite operator appeared on the right hand side of the evolution equation for the constraints, the method proposed here generates a general term of the correct sign which is added to terms of unknown sign that come from the underlying formalism. Under special circumstances, Detweiler showed that his method does in fact generate a negative-definite operator by making use of a free parameter introduced in his correction terms. The method proposed here also uses a free parameter in arguing that the constraints can be evolved toward zero, with the difference that the argument here is more general but without a guarantee that the overall sign of the constraint evolution has the correct sign.

The A-system approach, proposed by Brodbeck, Frittelli, Hübner, and Reula, embeds the Einstein equations into a larger system of symmetric hyperbolic equations. The Einstein equations are coupled to the larger system by adding terms to the Einstein evolution equations which are zero on the constraint hypersurface, with the extra degrees of freedom defined such that they are forever zero if the Einstein constraints and constraints on the new degrees of freedom are satisfied in the initial data. A linear order analysis of this system suggests that for “small enough” deviations from the constraint hypersurface, the system should asymptote to a solution of the Einstein equations.

Finally, Yoneda and Shinkai [9] performed detailed eigenvalue calculations to determine the theoretical signs of the constraint evolution when linearizing around a Minkowski background spacetime. While their program was intensive and thorough, their results depend on the validity of a perturbation expansion around a fixed space-time. In that limit, they evaluate the sign of the eigenvalues of their expansion matrix, and use those signs to predict the goodness of correction terms which are strictly linear in the constraints and spatial derivatives of the constraints. Although one of their more promising terms was used to good effect in a numerical experiment [10], their analysis remains strictly valid only in the perturbation regime around Minkowski space, and, at present, they have only examined terms linear in the constraints and derivatives of the constraints.

The method here, in contrast, attempts to make the constraint surface an attractor for the evolution equations without appealing to perturbation theory in any way and without extending the system of equations. The results will show it successful in reaching this goal for the simple case of the Maxwell equations, but cannot confirm with certainty that the results will generalize to nonlinear general relativity. The primary problem is that the correction terms proposed here have the form

$$\frac{d}{dt} \text{constraint}^2 = (\text{orig rhs}) - (\text{correction})$$

with a correction term of definite sign subtracted from a
term of indefinite sign coming from the underlying theory. The success of the method in the case of the linear Maxwell equations makes a similar result in the linearized Einstein equations likely, but does not guarantee success for full, non-linear general relativity. This will be discussed more completely in Section IV.

In this paper, following earlier work by Knapp, Walker, and Baumgarte (KWB) [11], I will apply the method to Maxwell’s equations as a proof-of-concept test. The work by KWB showed that some qualitative features of two popular ADM formulations of general relativity are manifest in the simpler framework of electromagnetism, making this a natural place to demonstrate the feasibility of the new methods presented here.

II. THE THEORY

I will introduce the idea here by first considering the ordinary differential equation example of the simple harmonic oscillator, and then considering the more interesting case of partial differential equations.

A. ODE: Harmonic Oscillator

The equations of motion for a harmonic oscillator (with \( \omega = 1 \)) are

\[
\frac{dx}{dt} = v \\
\frac{dv}{dt} = -x
\]

(1) (2)

and the constraint \( E \) is the shifted energy function

\[
E(t) = x^2 + v^2 - E_0
\]

(3)

with \( E_0 = x^2(0) + v^2(0) \), which should be zero-valued at all times. In a numerical evolution, one would like to evolve the fundamental quantities \( x \) and \( v \), and, after doing so, calculate the constraint \( E(t) \) from \( x \) and \( v \). Since \( E \) is derived, on the other hand, it makes sense to look at its time evolution in terms of the time evolution of \( x \) and \( v \) using the chain rule. Furthermore, \( E(t) \) is not bounded on either side, so consider instead \( E^2(t) \), which should also always be zero. Applying the chain rule gives the elementary result that

\[
\frac{dE^2}{dt} = F(x,v) = \frac{\partial E^2}{\partial x} \frac{dx}{dt} + \frac{\partial E^2}{\partial v} \frac{dv}{dt}.
\]

(4)

Now we cannot change the two partial derivative factors since they are fixed by the form of the energy expression, but, as noted before, we are free to change the equations of motion without changing the physics by adding multiples of the constraints. Let \( K \) be a positive constant. If we make the changes

\[
\frac{dx}{dt} = v - K \frac{\partial E^2}{\partial x}
\]

(5)

\[
\frac{dv}{dt} = -x - K \frac{\partial E^2}{\partial v}
\]

(6)

to the equations of motion, then

\[
\frac{dE^2}{dt} = F(x,v) - K \left[ \left( \frac{\partial E^2}{\partial x} \right)^2 + \left( \frac{\partial E^2}{\partial v} \right)^2 \right]
\]

(7)

shows how the constraint evolves under the new equations of motion. For large \( K \), the term in brackets will dominate the evolution of the constraint, constantly pushing it toward its minimum value of zero.

Numerical results, integrating forward in time with the Euler method, are in agreement with this analytic result.

B. PDEs

Having seen the method in the simple case of ODEs, consider now the the more interesting case of PDEs with one constraint equation. Let \( s \) be the state vector for a system. Define

\[
S_m(t,x) = \frac{\partial s_m}{\partial t}
\]

(8)

to be the right hand side of the evolution equation in the unmodified formalism. A general constraint \( C \) will depend on \( s \) and its spatial derivatives. Furthermore, the constraint should be satisfied at every point in space. These considerations motivate looking at the integrated, squared constraint \( C^2 = \int C^2 d^N x \), and, instead of taking partial derivatives with respect to the fields, we need to take variational derivatives of the integrated constraint when considering the analogies of Equations (5–6) so that the dependence of \( C \) on the spatial derivatives of the fields is treated properly.

Following this prescription, the appropriate modification to the equation of motion for the state vector is

\[
\frac{\partial s_m}{\partial t} = S_m(t,x) - K_{mn}(t,x) \frac{\delta C^2}{\delta s_n(t,x)}
\]

(9)

for some positive-definite matrix-valued function \( K_{mn} \). Under this change,

\[
\frac{dC^2}{dt} = D[s] - \int \left( \frac{\delta C^2}{\delta s_m} \right) K_{mn} \left( \frac{\delta C^2}{\delta s_n} \right) d^N x
\]

(10)

gives the evolution of the constraint in the modified theory. Here \( D[s] \) gives the functional form of the right hand side of the constraint’s evolution equation in the unmodified theory. For the cases considered here, I chose the \( K_{mn} \) diagonal and constant.

For systems with \( M \) constraint equations, the method is easily modified by taking the grand constraint functional to be

\[
\overline{C}_G^2 = \int w_{IJ}(t,x) C_I C_J d^N x
\]

(11)
with any positive definite matrix $w_{ij}$. Like $K_{mn}$, the matrix $w_{ij}$, can, in principle, be a function of both space and time, and can have off-diagonal entries. In practice, however, I have only used diagonal and constant matrices. Even in the diagonal case, the matrix is necessary because there is no a priori reason to believe that the constraints have the same dimensions, and it also allows the different constraints to be treated with different relative importance. In addition, since there is no natural scale for the grand constraint, one may always set one of the coefficients $w_{ij}$ in (11) to unity.

III. APPLICATION TO MAXWELL

This section takes Maxwell’s equations as a concrete example of a system of partial differential equations subject to a pointwise constraint. Following KWB [11], I consider two ways of writing Maxwell’s equations for the vacuum in terms of the vector potential $A_i$. The first system, called System I, uses the evolution equations

\[
\begin{align*}
\partial_t A_i &= -E_i - \partial_t \psi \\
\partial_t E_i &= -\partial_j \partial_j A_i + \partial_i \partial_j A_j
\end{align*}
\]  

(12) and (13)

and the constraint

\[
C_E = \partial_t E_i = 0.
\]  

(14)

The second system introduces the additional field $\Gamma$ defined by

\[
\Gamma = \partial_t A_i
\]  

(15)

to eliminate mixed derivatives in (13). The evolution equations for System II are

\[
\begin{align*}
\partial_t E_i &= -\partial_j \partial_j A_i + \partial_i \Gamma \\
\partial_t \Gamma &= -\partial_i \partial_i \psi
\end{align*}
\]  

(16) and (17)

and (12). Both systems use a gauge consistent with

\[
\partial_i \psi = -\partial_i A_i = -\Gamma
\]  

(18)

using the first equality for System I and the second for System II.

A. System I Evolution Equations

Having defined the systems, I would now like to calculate the terms required for applying the constraint finding method to System I. Here there is only one constraint, $C = C_E = \partial_t E_i$, which is zero-valued. It depends only on the first derivatives of the electric field, therefore I need only to calculate

\[
\frac{\delta C^2}{\delta E_i(x)} = -2\partial_i C_E
\]  

(19)

which modifies (13). The new evolution equation for the electric field is

\[
\partial_t E_i = -\partial_k \partial_k A_i + \partial_i \partial_k A_k + 2K_E \partial_i C_E
\]  

(20)

for an arbitrary positive $K_E$, while the other System I evolution equations (12) and (18) remain unchanged.

B. System II Evolution Equations

System II, unlike System I, has two constraints that should be enforced, the original constraint given by (14) plus the definition of $\Gamma$ in (15), rewritten as

\[
C_\Gamma = \partial_t A_i - \Gamma = 0
\]  

(21)

to make it zero-valued. This provides more freedom in constructing the grand constraint

\[
C^2 = C_E^2 + wC_\Gamma^2
\]  

(22)

where one does not necessarily have to treat the constraints on equal footing. In this case, the total constraint depends additionally on $\Gamma$ and first derivatives of the vector potential. In addition to (19), which is still valid, I need

\[
\frac{\delta C^2}{\delta A_i(x)} = -2w\partial_i C_\Gamma
\]  

(23)

\[
\frac{\delta C^2}{\delta \Gamma(x)} = -2wC_\Gamma
\]  

(24)

to enforce the definition of $\Gamma$.

Applying these correction terms to the evolution equations gives the new equations of motion

\[
\begin{align*}
\partial_t A_i &= -E_i - \partial_t \psi + 2wK_A \partial_i C_\Gamma \\
\partial_t E_i &= -\partial_k \partial_k A_i + \partial_i \Gamma + 2K_E \partial_i C_E \\
\partial_i \Gamma &= -\partial_k \partial_k \psi + 2wK_\Gamma C_\Gamma
\end{align*}
\]  

(25) and (26) and (27)

which, combined with (18), form a complete system. The constants $K_A$ and $K_\Gamma$ are arbitrary but positive.

C. Propagation of Constraints

In [11], KWB examined the evolution equation for $C_E$ in both systems. They showed that for System I, the constraint does not evolve in time, and that in System II, the constraint obeys a wave equation. They did not have reason, however, to consider the time evolution of the secondary constraint $C_\Gamma$. I extend their results here by showing that the secondary constraint also satisfies a wave equation in the unmodified case. Furthermore, I demonstrate the improved behavior of the constraints under the modifications proposed here.

Calculating the first time derivatives of the constraints is easily accomplished by taking the time derivatives of
and replacing the time derivatives that appear on the right hand sides of the equations by the evolution equations \((28)\), \((29)\), and \((30)\). This gives the results

\[
\begin{align*}
\partial_t C_E &= -\partial_t^2 \left[ C_T - 2 K_E C_E \right] \\
\partial_t C_T &= -C_E + 2 \omega \left[ K_A \partial_t^2 C - K_T C_T \right]
\end{align*}
\]

which can be viewed as valid for both systems if \(C_T\) is taken to be identically zero for System I.

To see that KWB have a wave equation for the secondary constraint, set all of the \(K\)'s to zero in \((28)\) and \((29)\) to eliminate the modifications, and take the time derivative of \((28)\). The result

\[
\partial_t^2 C_T = \partial_t^2 C_T
\]

follows immediately.

Of greater interest here, however, is an analysis on the modified equations \((28)\), \((29)\) in their first derivative form. The equations are linear, so they admit a Fourier analysis by substituting a plane wave solution \(e^{i k x}\) into the right hand sides. After substituting, the resulting equations

\[
\begin{align*}
\partial_t C_E &= k^2 C_T - 2 K_E k^2 C_E \\
\partial_t C_T &= -C_E - 2 \omega \left[ K_A k^2 + K_T \right] C_T
\end{align*}
\]

retain the terms that gave the KWB wave equations for the constraints, but have additional terms that look like they provide exponential decay. This system of equations is, in fact, simple enough for Maple to solve analytically for general values of the \(K\)'s in one dimension. The solution, which is too long to display in detail here, consists of a sum of terms with the form

\[
\exp \left[ \left( -f_1^+ \pm \sqrt{\sigma \left( f_1^+ \right)^2 - k^2} \right) t \right] f_2
\]

where

\[
f_1^+ \left( k^2 \right) = \left( K_E \pm w K_A \right) k^2 \pm w K_T
\]

\(\sigma = \pm 1\), and \(f_2 = f_2(k, C_0(0, x))\) is some simple function of \(k\) and the initial values of the constraints. Since \(f_1^+ \left( k^2 \right) > 0\) is manifestly positive and the radical is either positive or pure imaginary, the only term of this form that could cause anything other than exponential decay is \(-f_1^+ + \sqrt{\sigma \left( f_1^+ \right)^2 - k^2}\) for parameters where \(\sigma \left( f_1^+ \right)^2 - k^2 > 0\). Simple algebraic analysis, however, shows that even this term has an overall minus sign, giving exponential decay.

In order to make the argument more concrete, I present here the \(k = 1\) solution

\[
\begin{align*}
C_E(t, x) &= e^{-3t} \left[ C_E(0, x) + S(x)t \right] \quad (35) \\
C_T(t, x) &= e^{-3t} \left[ C_T(0, x) - S(x)t \right]
\end{align*}
\]

for which all of the \(K\)'s are set equal to one. Here \(S(x) = C_E(0, x) + C_T(0, x)\) is a short hand. The general solution can be requested from the author in the form of a Maple worksheet.

My numerical experiments on these modified systems of equations used an ICN integration scheme \([12]\), and a Courant factor of 1/2. The spatial domain ran from -6 to +6, with data stored on 99 points in each coordinate direction. On the evolved fields \((E_1, A_1, \psi_1, \Gamma)\), I imposed outgoing wave boundary conditions (see \([12]\) for implementation details), and on the constraints, I imposed \(C_T = 0\) for applicable \(I\). All runs were performed on a 500 MHz Digital Personal Workstation with 1.5 GB of RAM.

For each system, I ran three parameter sets, one of which reproduced the equations used by KWB. The full definitions of all of the parameter sets are found in Table I. Sensible values of the parameters were easily determined by trial and error. Choosing the values too small, as expected, makes little difference in the evolution, while choosing the values too large leads to numerical instabilities during the transient period of the evolution \([16]\).

I followed KWB in using the analytic solution

\[
\begin{align*}
A^\phi &= 0 \\
E^\phi &= 8 \lambda^2 r e^{-\lambda r^2} \sin \theta
\end{align*}
\]

of a toroidal dipole to generate the initial data. The other components of the fields are zero. I chose \(\lambda = A = 1\), and the conversion from spherical to Cartesian coordinates was made in the code.

The results of the System I runs are summarized in Figure I, which shows a plot of \(\| C_E \|_2\) vs. \(t\). The I-0 (control) curve reproduces the findings of KWB that, after an initial transient, the \(C_E\) constraint does not evolve in time. The I-1 and I-2 curves, representing different values (see Table I) of the parameter \(K_E\), on the other hand, show a modulated exponential decay. Eventually, around \(t \approx 200\), the I-1 case also stops decaying as rapidly, while the rapid exponential decay continues through the end of the run for I-2.

That the constraint in the modified case I-1 ceases to evolve at some point is consistent with \([10]\), which implies that the constraints will cease to evolve when the first term balances with the second term. From \([10]\), one expects that this balance will be achieved for smaller constraint violation when the driving parameter is larger, which is consistent with the results shown in Figure I.

### Table I: The parameters used for the various data runs done on the two Maxwell systems are tabulated here.

| Run | \(K_E\) | \(K_A\) | \(K_T\) | \(w\) |
|-----|--------|--------|--------|------|
| I-0 | 0      | -      | -      | -    |
| I-1 | \(1 \times 10^{-2}\) | -      | -      | -    |
| I-2 | \(5 \times 10^{-2}\) | -      | -      | -    |
| II-0| 0      | 0      | 0      | 1    |
| II-1| \(5 \times 10^{-3}\) | \(5 \times 10^{-3}\) | \(5 \times 10^{-3}\) | 1    |
| II-2| \(1 \times 10^{-2}\) | \(1 \times 10^{-2}\) | \(1 \times 10^{-2}\) | 1    |
Looking at two dimensional slices of the constraint data at various times, also suggests that the source of the modulation in the decay demonstrated by I-1 and I-2 is fluctuations at the boundary, possibly caused by the simple boundary condition applied there on the constraints. Significantly, these fluctuations are unable to penetrate the interior of the computational domain, unlike many scenarios seen in experimental relativity where noise from the boundary noticeably propagates inward from the outer boundary, eventually killing the simulation. Because I am only interested in the Maxwell equations as a test-bed for the method, and because the modified System I equations already perform orders of magnitude better than their unmodified counterpart, I have not pursued this point further.

Figure 2 shows a plot of $\|C_E\|_2$ vs. $t$ for the System II case. Here again, the control run (II-0) reproduces the results of KWB, this time showing exponential decay in the primary constraint. Even with such an ideal result in the unmodified case, the modified runs II-1 and II-2 show improvement. They represent runs with non-zero values (see Table I) of the various forcing parameters, and in these cases the constraint decays exponentially, but with a smaller characteristic time.

Figure 3 is a plot of $\|C_\Gamma\|_2$ versus time $t$, and shows similar behavior to the primary constraint in all three cases. The secondary constraint shows exponential decay in the unmodified II-0 case, while showing a faster decay in the two modified runs, II-1 and II-2. The jump in the graph at $t = 0$ occurs because the secondary constraint is exactly satisfied in the initial data by construction.

It should be noted that one likely explanation for the extremely favorable performance of the unmodified System II is that, since the constraints satisfy a wave equation, constraint violations propagate off of the grid. This is supported by the data presented by KWB, showing that decay rate of the constraint decreases when the outer boundary is moved farther out [11]. The method presented here benefits from constraint violations propagating off of the grid as well, but, in addition, attempts to damp the constraint violation throughout the grid at all times.

In both systems, there is a practical limit to how large the forcing parameters may be chosen without creating an instability. I believe that its origin can be seen in (33), which shows how the dispersion relation for the Fourier components of the solutions is modified by the new terms. This modification is effectively a modification of the propagation speed of those components, which, for a fixed Courant factor, can lead to numerical instabilities in the numerical scheme. When the forcing parameters are too large, the code crashes. The constraint blows up rapidly immediately before such a crash, and such crashes usually occur during the transient period of the numerical scheme.

IV. CONCLUSIONS AND DISCUSSION

The method proposed here does not provide a formalism for any physical system. It attempts to take any formalism and makes that formalism better. The analy-
sis does not depend on the form of the equations and the arguments leading to the modifications do not depend on the validity of any perturbative expansion. The results in the case of the Maxwell equations are very encouraging and consistent with the analytic predictions. Should the results derived from Maxwell’s equations generalize to the Einstein equations, furthermore, this could prove extremely beneficial to the long term stability of simulations in numerical relativity. Fourier analysis of the ADM system suggests that instabilities seen in various 3+1 formulations are triggered by exponentially growing modes not seen in the initial data \[1\]. On the other hand, at least for the case of the Maxwell equations, the terms added via the method proposed here lead to exponential damping terms in the evolution equations for all Fourier modes.

It should be noted, however, that in some sense the Maxwell equations were an optimal case. Notice, by counting the number of integrations by parts required to calculate the correction terms to the evolution equations, that the highest order of spatial derivatives in the new evolution equations will be the larger of (1) order of the original equations and (2) twice the order of the constraints. This means that, while the order of the Maxwell evolution equations was not changed, the Einstein equations will change from second order to fourth order in space. How this change of order effects the numeric solutions to the equations must be studied as this method is applied in the context of numerical relativity.

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FIG. 3: The $l_2$ norm of the secondary constraint $C_\Gamma$ versus time $t$ for three test cases. Case II-0 is the result of KWB. See Table I for other parameter values. At $t = 0$ the constraint is identically satisfied.

\[\begin{align*}
\text{System II: } ||C_\Gamma||_2 &\text{ vs. } t \\
\end{align*}\]

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[15] This is actually a conserved quantity. For this simple ODE case, there is no difference, but when we pass to PDEs, there will be a difference between conserved quantities and constraints.
[16] One possible explanation for the instability associated with large parameters is that the added terms modify the dispersion relationships for the various Fourier modes, as seen in \[13\]. Large values of the parameters may require adjustments to the Courant condition, which has not been analyzed here.