Formulations of the Einstein Equations for Numerical Simulations

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We review recent efforts to re-formulate the Einstein equations for fully relativistic numerical simulations. The so-called numerical relativity is a promising research field matching with ongoing gravitational wave observations. In order to complete long-term and accurate simulations of binary compact objects, people seek a robust set of equations against the violation of constraints. Many trials have revealed that mathematically equivalent sets of evolution equations show different numerical stabilities in free evolution schemes. In this article, we overview the efforts of the community, categorizing them into three directions: (1) modifying of the standard Arnowitt-Deser-Misner (ADM) equations initiated by the Kyoto group [the so-called Baumgarte-Shapiro-Shibata-Nakamura (BSSN) equations], (2) rewriting the evolution equations in a hyperbolic form and (3) constructing an "asymptotically constrained" system. We then introduce our series of works that try to explain these evolution behaviors in a unified way by using an eigenvalue analysis of the constraint-propagation equations. The modifications of (or adjustments to) the evolution equations change the character of constraint propagation and several particular adjustments using constraints are expected to damp the constraint-violating modes. We show several sets of adjusted ADM and BSSN equations, together with their numerical demonstrations.

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I. INTRODUCTION

1. Overview

The theory of general relativity describes the nature of the strong gravitational field. The Einstein equation predicts quite unexpected phenomena, such as gravitational collapse, gravitational waves, the expanding universe and so on, which are all attractive not only for researchers but also for the public. The Einstein equation consists of 10 partial differential equations (elliptic and hyperbolic) for 10 metric components and it is not easy to solve them for any particular situation. Over the decades, people have tried to study the general-relativistic world by finding its exact solutions, by developing approximation methods, or by simplifying the situations. While "The Exact Solution" book [1] says there were more than 4000 publications on exact solutions between 1980 and 2000, direct numerical integration of the Einstein equations can be said to be the most robust way to study the strong gravitational field. This research field is often called "numerical relativity."

With the purpose of predicting precise gravitational waveforms from coalescences of binary neutron-stars and/or black-holes, numerical relativity has been developed over the past three decades. The difficulty of numerical integrations of the Einstein equations arises from the mathematical complexity of the equations, the physical difficulty of singularity treatments and high-level requirements for computational skills and technology.

In 2005-2006, several groups independently announced that simulations of the inspiral black-hole binary merger were available [2-6]. There are many implements for their successes, such as gauge conditions, coordinate selections, boundary treatments, singularity treatments, numerical discretization and mesh refinements, together with the re-formulation of the Einstein equations which we will discuss here. More general and recent introductions to numerical relativity are available, e.g. those by Baumgarte-Shapiro (2003) [7], Alcubierre (2004) [8], Pretorius (2007) [9] and Bruegmann (2008) [10].

The purpose of this article is to review the formulation problem in numerical relativity. This is one of the essential issues to achieve long-term stable and accurate simulations of binary compact objects. Mathematically equivalent sets of evolution equations show different numerical stabilities in free evolution schemes. This had been a mystery for a long time between relativists and many proposals and trials were reported. After we review the problem from such a historical viewpoint, we
will explain our systematic understanding by using the constraint propagation equations; the evolution equations of the constraints which is supposed to be satisfied all through the time evolutions.

Most numerical relativity groups today use the so-called BSSN (Baumgarte-Shapiro-Shibata-Nakamura) equations, which represents a modified form of the ADM (Arnowitt-Deser-Misner) equations. We try to explain why these differences appear. We also predict that more robust sets of equations exist and give actual numerical demonstrations.

2. Formulation Problem in Numerical Relativity

There are several different approaches to simulating the Einstein equations. Among them, the most robust way, which we target in this article, is to apply $3 + 1$ (space + time) decomposition of space-time. This formulation was first given by Arnowitt, Deser and Misner (ADM) [11] (we call this the original ADM system, hereafter) with the purpose of constructing a canonical formulation of the Einstein equations to seek the quantum nature of space-time. In the late 70s, when numerical relativity started, this ADM formulation was introduced by Smarr and York [18,19] in slightly different notations which is taken as the standard formulation between numerical relativists (we call this the standard ADM system, hereafter).

The ADM formulation divides the Einstein equations into constraint equations and evolution equations, like the Maxwell’s equations. Since the set of ADM equations form a first-class system, if we solved two constraint equations, the Hamiltonian (or energy) constraint and the momentum constraint equations for the initial data, then the set of evolution equations theoretically guarantees that the evolved data will satisfy the constraint equations. This free-evolution approach is also the standard in numerical relativity, because solving the constraints (non-linear elliptic equations) is numerically expensive and because the free-evolution allows us to monitor the accuracy of the numerical evolution by using the constraint equations.

Up to the middle of the 90s, ADM numerical relativity had appealed great successes. For example, the formation of naked singularity from collisionless particles [12] shows the unknown behavior of the strong gravity; the discovery of the critical behavior for a black-hole formation [13] open-doors to the understanding of phase-transition nature in general relativity; the black-hole horizon dynamics [14] realized theoretical predictions.

Nevertheless, when people try to make long-term simulations, such as coalescences of neutron-star binaries and/or black-hole binaries for calculating gravitational-wave form, numerical simulations were often interrupted by unexplained blow-ups or divergences (Figure 1). This was thought to be due to the lack of resolution, inappropriate gauge choice, or the particular numerical scheme that was applied. However, with the accumulation of experience, people have noticed the importance of the formulation of the evolution equations, because there are apparent differences in numerical stability although the equations are mathematically equivalent.

At this moment, there are three major ways to obtain longer time evolutions, which we describe in the next section. Of course, the ideas, procedures and problems are mingled with each other. The purpose of this article is to review all three approaches and to introduce our idea to view them in a unified way. The author wrote a detail review of this topic in 2002 [15] and the present article includes an update in brief style.

The word stability is used in quite different ways in the community.

- We mean by numerical stability a numerical simulation which continues without any blow-ups and in which data remain on a constrained surface.

- Mathematical stability is defined in terms of the well-posedness in the theory of partial differential equations, such that the norm of the variables is bounded by the initial data. See Eq. (28) and the following paragraphs.
• For numerical treatments, there is also another notion of stability, the stability of finite differencing schemes. This means that numerical errors (truncation, round-off, etc.) do not grow by evolution. The evaluation is obtained using von Neumann’s analysis. Lax’s equivalence theorem says that if a numerical scheme is consistent (converging to the original equations in its continuum limit) and stable (no error growth), then the simulation represents the right (converging) solution. See Ref. [16] for the Einstein equations.

We follow the notations of Misner-Thorne-Wheeler [17]. We use \( \mu, \nu = 0, \cdots, 3 \) and \( i, j = 1, \cdots, 3 \) as space-time indices. The unit c = 1 is applied. The discussion is mostly for the vacuum space-time, but the inclusion of matter is straightforward.

II. THE STANDARD WAY AND THE THREE OTHER ROADS

1. Strategy 0: The ADM formulation

A. The original ADM formulation

The Arnowitt-Deser-Misner (ADM) formulation [11] gave the fundamental idea of time evolution of space and time: such as foliations of 3-dimensional hypersurface \( \Sigma \) (Figure 2). The story begins by decomposing 4-dimensional space-time into 3 plus 1. The metric is expressed by

\[
ds^2 = g_{\mu \nu} dx^\mu dx^\nu = -\alpha^2 dt^2 + \gamma_{ij}(dx^i + \beta^i dt)(dx^j + \beta^j dt),
\]

where \( \alpha \) and \( \beta \) are defined as \( \alpha \equiv 1/\sqrt{-g_{00}} \) and \( \beta \equiv g_{0i} \), and are called the lapse function and the shift vector, respectively. The projection operator or the intrinsic 3-metric \( g_{ij} \) is defined as \( \gamma_{\mu \nu} = g_{\mu \nu} + n_\mu n_\nu \), where \( n_\mu = (-\alpha, 0, 0) \) [and \( n^\mu = g^{\mu \nu} n_\nu = (1/\alpha, -\beta/\alpha) \)] is the unit normal vector of the spacelike hypersurface, \( \Sigma \) (see Figure 2). By introducing the extrinsic curvature,

\[
K_{ij} = -\frac{1}{2} \tilde{\mathcal{L}} n \gamma_{ij},
\]

and using the Gauss-Codacci relation, the Hamiltonian density of the Einstein equations can be written as

\[
\mathcal{H}_{GR} = \pi^{ij} \gamma_{ij} - \mathcal{L},
\]

where

\[
\mathcal{L} = \sqrt{-g} R = \alpha \sqrt{\gamma} (R^{(3)} - K^2 + K_{ij} K^{ij}),
\]

with \( \pi^{ij} \) being the canonically conjugate momentum to \( \gamma_{ij} \),

\[
\pi^{ij} = \frac{\partial \mathcal{L}}{\partial \dot{\gamma}_{ij}} = -\sqrt{\gamma} (K^{ij} - K \gamma^{ij}),
\]

omitting the boundary terms. The variation of \( \mathcal{H}_{GR} \) with respect to \( \alpha \) and \( \beta_i \) yields the constraints and the dynamical equations are given by \( \gamma_{ij} = \frac{\delta \mathcal{H}_{GR}}{\delta \pi^{ij}} \) and \( \pi^{ij} = -\frac{\delta \mathcal{H}_{GR}}{\delta h_{ij}} \).

B. The standard ADM formulation

In the version of Smarr and York [18, 19], \( K_{ij} \) was used as a fundamental variable instead of the conjugate momentum \( \pi^{ij} \). The set of equation is summarized as follows:

The Standard ADM formulation [18, 19]

The fundamental dynamical variables are \( (\gamma_{ij}, K_{ij}) \), the three-metric and the extrinsic curvature. The three-hypersurface \( \Sigma \) is foliated with gauge functions, \( (\alpha, \beta^i) \), the lapse and the shift vector.

• The evolution equations:

\[
\partial_t \gamma_{ij} = -2\alpha K_{ij} + D_i \beta_j + D_j \beta_i, \tag{6}
\]

\[
\partial_t K_{ij} = \alpha (3) R_{ij} + \alpha KK_{ij} - 2\alpha K_{ik} K^{kj} - D_i D_j \alpha + (D_i \beta^k) K_{kj} + (D_j \beta^k) K_{ki} + \beta^k D_k K_{ij}, \tag{7}
\]

where \( K = K^i_i \) and \( (3) R_{ij} \) and \( D_i \) denote the three-dimensional Ricci curvature and a covariant derivative on the three-surface, respectively.

• Constraint equations:

\[
\mathcal{H}^{ADM} := (3) R + K^2 - K_{ij} K^{ij} \approx 0, \tag{8}
\]

\[
\mathcal{M}_A^{ADM} := D_j K_{ij} - D_i K \approx 0, \tag{9}
\]

where \( (3) R \equiv (3) R^i_i \); these are called the Hamiltonian (or energy) and momentum constraint equations, respectively.
The formulation has 12 first-order dynamical variables $(\gamma_{ij}, K_{ij})$, with 4 freedom of gauge choices $(\alpha, \beta_i)$ and with 4 constraint equations, Eqs. (8) and (9). The rest freedom expresses two modes of gravitational waves.

We remark that there is one replacement in Eq. (7) by using Eq. (8) in the process of conversion from the original ADM to the standard ADM equations. This is the key issue in the later discussion and we shall come back to this point in Section II.2.

The constraint propagation equations, which are the time evolution equations of the Hamiltonian constraint, Eq. (8) and the momentum constraints, Eq. (9), can be written as follows:

**Constraint Propagations of the Standard ADM:**

\[
\begin{align*}
\partial_t H &= \beta^i (\partial_i H) + 2\alpha K H - 2\alpha \gamma^{ij} (\partial_i M_j) \\
&\quad + \alpha (\partial_i \gamma_{mk}) (2\gamma^{ml} \gamma^{kj} - \gamma^{mk} \gamma^{lj}) M_j \\
&\quad - 4\gamma^{ij} (\partial_i \alpha) M_i ,
\end{align*}
\]

\[
\begin{align*}
\partial_t M_i &= -(1/2) \alpha (\partial_i H) - (\partial_i \alpha) H + \beta^j (\partial_j M_i) \\
&\quad + \alpha K M_i - \beta^k \gamma^{ij} (\partial_i \gamma_{lk}) M_j + (\partial_i \beta_k) \gamma^{kj} M_j .
\end{align*}
\]

From these equations, we know that if the constraints are satisfied on the initial slice $\Sigma$, then the constraints are satisfied throughout the evolution. The normal numerical scheme is to solve the elliptic constraints for preparing the initial data and to apply the free evolution (solving only the evolution equations). The constraints are used to monitor the accuracy of the simulations.

The ADM formulation was the standard formulation for numerical relativity up to the middle 90s. Numerous successful simulations were obtained for the problems of gravitational collapse, critical behavior, cosmology and so on. However, stability problems have arisen for simulations such as the gravitational radiation from compact binary coalescence because the models require quite a long-term time evolution.

The origin of the problem was that the above statement in *italics* is true in principle, but is not always true in numerical applications. A long history of trial and error began in the early 90s. From the next subsection, we shall look back on them by summarizing “three strategies.” We then unify these three roads as “adjusted systems,” and as its by-product, we show that the standard ADM equations have a constraint violating mode in the constraint propagation equations even for a single black-hole (Schwarzschild) spacetime [71]. Figures 3 and 4 are chronological maps of the research.

2. Strategy 1: Modified ADM formulation by Nakamura et al. (The BSSN formulation)

Up to now, the most widely used formulation for large-scale numerical simulations has been the modified ADM
system, which is now often cited as the Baumgarte-Shapiro-Shibata-Nakamura (BSSN) formulation. This re-formulation was first introduced by Nakamura et al. [20–22]. The usefulness of this re-formulation was re-introduced by Baumgarte and Shapiro [23] and was then confirmed by other groups to show a long-term stable numerical evolution [24,25].

A. Basic variables and equations

The widely used notation [23] introduces the variables $(\varphi, \tilde{\gamma}_{ij}, K, \tilde{A}_{ij}, \tilde{\Gamma}^i)$ instead of $(\gamma_{ij}, K_{ij})$, where

$$\varphi = \frac{1}{12} \log(\det \gamma_{ij}),$$

$$\tilde{\gamma}_{ij} = e^{-4\varphi} \gamma_{ij},$$

$$K = \gamma^{ij} K_{ij},$$

$$\tilde{A}_{ij} = e^{-4\varphi} (K_{ij} - (1/3) \gamma_{ij} K),$$

$$\tilde{\Gamma}^i = \tilde{\Gamma}^{ij}_{jk} \delta^i_k.$$  

The new variable $\tilde{\Gamma}^i$ is introduced in order to calculate the Ricci curvature more accurately. In the BSSN formulation, the Ricci curvature is not calculated as $R^{ADM}_{ij} = \partial_k \Gamma^k_{ij} - \partial_i \Gamma^k_{kj} + \Gamma^k_{ij} \Gamma^l_{kl} - \Gamma^k_{ij} \Gamma^l_{kl}$, but as $R^{BSSN}_{ij} = R^{ADM}_{ij} + \tilde{R}_{ij}$, where the first term includes the conformal factor $\varphi$ while the second term does not. These are approximately equivalent, but $R^{BSSN}_{ij}$ apparently does have a wave operator in the flat background limit so that we can expect a more natural wave propagation behavior.

Additionally, the BSSN requires us to impose the conformal factor as $\tilde{\gamma} := \det \tilde{\gamma}_{ij} = 1$ during evolution. This is a kind of definition, but can also be treated as a constraint.

The BSSN formulation [20–23]:

The fundamental dynamical variables are $(\varphi, \tilde{\gamma}_{ij}, K, \tilde{A}_{ij}$ and $\tilde{\Gamma}^i)$. The three-hypersurface $\Sigma$ is foliated with gauge functions $(\alpha, \beta^i)$, the lapse and the shift vector.

- The evolution equations:

  $$\partial_t \varphi = -(1/6) \alpha K + (1/6) \beta_i (\partial_i \varphi) + (\partial_i \beta^k),$$

  $$\partial_t \tilde{\gamma}_{ij} = -2 \alpha \tilde{A}_{ij} + \tilde{\gamma}_{ik} (\partial_i \beta^k) + \beta_k (\partial_i \beta^k) - (2/3) \tilde{\gamma}_{ij} (\partial_k \beta^k) + \beta^k (\partial_k \tilde{\gamma}_{ij}),$$

  $$\partial_t \tilde{A}_{ij} = -(1/6) \alpha \tilde{B} + \alpha \tilde{A}_{ij} \tilde{A}^{ij} + (1/3) \alpha K^2 + \beta_i (\partial_i K),$$

  $$\partial_t \tilde{\Gamma}^i = -(1/6) \alpha \tilde{B} \tilde{A}_{ij} + (\partial_i \beta^k) \tilde{A}_{kj} + (\partial_k \beta^i) \tilde{A}_{ij}.$$
The second effort to re-formulate the Einstein equations is to make the evolution equations reveal a first-order hyperbolic form explicitly. This is motivated by the expectations that the symmetric hyperbolic system has well-posed properties in its Cauchy treatment in many systems and that the boundary treatment can be improved if we know the characteristic speed of the system.

**Hyperbolic formulations**

We say that the system is a first-order (quasi-linear) partial differential equation system, if a certain set of (complex-valued) variables $u_\alpha$ $(\alpha = 1, \cdots, n)$ forms

\[
\partial_t u_\alpha = M^{\beta\alpha}(u) \partial u_\beta + N_\alpha(u),
\]

where $M$ (the characteristic matrix) and $N$ are functions of $u$, but do not include any derivatives of $u$. Further, we say the system is

- **a weakly hyperbolic system** if all the eigenvalues of the characteristic matrix are real,
- **a strongly hyperbolic system** (or a diagonalizable / symmetrizable hyperbolic system) if the characteristic matrix is diagonalizable (has a complete set of eigenvectors) and has all real eigenvalues and
- **a symmetric hyperbolic system** if the characteristic matrix is a Hermitian matrix.

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Eqs. (22) and (23) are the Hamiltonian and the momentum constraints (the “kinematic” constraints) while the latter three are “algebraic” constraints due to the requirements of the BSSN variables.

**B. Remarks, pros and cons**

Why is the BSSN better than the standard ADM? Together with numerical comparisons with the standard ADM case [25], this question has been studied by many groups using different approaches.

- Using numerical test evolutions, Alcubierre et al. [24] found that the essential improvement is in the process of replacing terms by the momentum constraints. They also pointed out that the eigenvalues of the BSSN evolution equations have fewer “zero eigenvalues” than those of ADM and they conjectured that the instability might be caused by these “zero eigenvalues.”

- Miller [26] reported that the BSSN had a wider range of parameters that gave stable evolutions in the von Neumann’s stability analysis.

- An effort was made to understand the advantage of the BSSN from the point of hyperbolization of the equations in the linearized limit [24,27] or with a particular combination of slicing conditions plus auxiliary variables [28]. If we define the 2nd-order symmetric hyperbolic form, then the principal part of the BSSN can be one of them [29].

As we discussed in Ref. [30], the stability of the BSSN formulation is due not only to the introductions of new variables but also to the replacement of terms in the evolution equations by using constraints. Further, we can show several additional adjustments to the BSSN equations, which give us more stable numerical simulations. We will devote Section III. to this fundamental idea.

The current binary black-hole simulations apply the BSSN formulations with several implementations. For example,

\[-(2/3)(\partial_k b^k)\tilde{A}_{ij} + \beta^k(\partial_k \tilde{A}_{ij}), \tag{20}\]

\[
\partial_t \tilde{\Gamma}^i = -2(\partial_j \alpha)\tilde{A}^{ij} + 2\alpha(\tilde{\Gamma}^{ij}_{jk}b^k) - (2/3)\tilde{\gamma}^{ij}(\partial_j K) + 6\tilde{A}^{ij}(\partial_j \tilde{\gamma}) - \partial_j(\beta^k(\partial_k \tilde{\gamma}^{ij}) - \tilde{\gamma}^{ij}(\partial_k \beta^i)) - \tilde{\gamma}^{ki}(\partial_k \beta^i) + (2/3)\tilde{\gamma}^{ij}(\partial_k b^k)). \tag{21}\]

- **Constraint equations:**

\[\mathcal{H}^{BSSN} = R^{BSSN} + K^2 - K_{ij}K^{ij}, \tag{22}\]

\[\mathcal{M}^{BSSN}_i = \mathcal{M}^{ADM}_i, \tag{23}\]

\[G^i = \tilde{\Gamma}^i - \tilde{\gamma}^{jk}\tilde{\Gamma}^i_{jk}, \tag{24}\]

\[\mathcal{A} = \tilde{A}_{ij}\tilde{\gamma}^{ij}, \tag{25}\]

\[S = \tilde{\gamma} - 1. \tag{26}\]
Writing the system in a hyperbolic form is a quite useful step in proving that the system is well-posed. Mathematical well-posedness of the system means (1◦) local existence (of at least one solution $u$), (2◦) uniqueness (i.e., at most solutions), and (3◦) stability (or continuous dependence of solutions $\{u\}$ on the Cauchy data) of the solutions. The resultant statement expresses the existence of the energy inequality on its norm,

$$||u(t)|| \leq e^{\alpha t}||u(t=0)||,$$

where $0 < \tau < t$, $\alpha = \text{const}$. (28)

This indicates that the norm of $u(t)$ is bounded by a certain function and the initial norm. We remark that this mathematical bounds does not mean that the norm $u(t)$ decreases along the time evolution.

The inclusion relation of the hyperbolicities is

symmetric hyperbolic $\subset$ strongly hyperbolic $\subset$ weakly hyperbolic. (29)

The Cauchy problem under weak hyperbolicity is not, in general, $C^\infty$ well-posed. At the strongly hyperbolic level, we can prove the finiteness of the energy norm if the characteristic matrix is independent of $u$ (cf. [34]), that is, one step definitely advanced over a weakly hyperbolic form. Similarly, the well-posedness of the symmetric hyperbolic is guaranteed if the characteristic matrix is independent of $u$ while if it depends on $u$, we have only limited proofs for the well-posedness.

From the point of numerical applications, to hyperbolize the evolution equations is quite attractive, not only for its mathematically well-posed features. The expected additional advantages are the following:

(a) It is well known that a certain flux conservative hyperbolic system is taken as an essential formulation in the computational Newtonian hydrodynamics when we control shock wave formations due to matter.

(b) The characteristic speed (eigenvalues of the principal matrix) is supposed to be the propagation speed of the information in that system. Therefore, it is naturally imagined that these magnitudes are equivalent to the physical information speed of the model to be simulated.

(c) The existence of the characteristic speed of the system is expected to give us an improved treatment of the numerical boundary and/or to give us a new well-defined Cauchy problem within a finite region (the so-called initial boundary value problem; IBVP).

These statements sound reasonable, but have not yet been generally confirmed in actual numerical simulations in general relativity.

B. Hyperbolic formulations of the Einstein equations

Most physical systems can be expressed as symmetric hyperbolic systems. In order to prove that the Einstein’s theory is a well-posed system, to hyperbolize the Einstein equations is a long-standing research area in mathematical relativity.

The standard ADM system does not form a first-order hyperbolic system. This can be seen immediately from the fact that the ADM evolution equation, Eq. (7), has a Ricci curvature in the right-hand-side. This is also a common fact in the BSSN formulation.

So far, several first-order hyperbolic systems of the Einstein equation have been proposed. In constructing hyperbolic systems, the essential procedures are (1◦) to introduce new variables, normally the spatially derivative metric, (2◦) to adjust equations using constraints and occasionally (3◦) to restrict the gauge conditions and/or (4◦) to rescale some variables. Due to process (1◦), the number of fundamental dynamical variables is always larger than that of the ADM.

Due to the limitation of space, we can only list several hyperbolic systems of the Einstein equations:

- The Bona-Masso formulation [35,36]
- The Einstein-Ricci system [37, 38] / Einstein-Bianchi system [39]
- The Einstein-Christoffel system [40]
- The Ashtekar formulation [41,42]
- The Frittelli-Reula formulation [34,43]
- The Conformal Field equations [44]
- The Bardeen-Buchman system [45]
- The Kidder-Scheel-Teukolsky (KST) formulation [46]
- The Alekseenko-Arnold system [47]
- The general-covariant Z4 system [48]
- The Nagy-Ortiz-Reula (NOR) formulation [49]
- The Weyl system [50,51]

Note that there are no apparent differences between the word ‘formulation’ and ‘system’ here.

C. Numerical tests

When we discuss hyperbolic systems in the context of numerical stability, the following questions should be considered:
Q: From the point of the set of evolution equations, does hyperbolization actually contribute to numerical accuracy and stability? Under what conditions/situations will the advantages of hyperbolic formulation be observed?

Unfortunately, we do not have conclusive answers to these questions, but much experience is being accumulated. Several earlier numerical comparisons reported the stability of hyperbolic formulations [36,52–54], but we have to remember that this statement went against the standard ADM formulation.

These partial numerical successes encouraged the community to formulate various hyperbolic systems. However, several numerical experiments also indicate that this direction is not a complete success:

- Above earlier numerical successes were also terminated with blow-ups.
- If the gauge functions evolve according to the hyperbolic equations, then their finite propagation speeds may cause pathological shock formations in simulations [55,56].
- There are no drastic differences in the evolution properties between hyperbolic systems (weakly, strongly and symmetric hyperbolicity) for the systematic numerical studies by Hern [57] based on Frittelli-Reula formulation [43] and by the authors [58] based on Ashtekar’s formulation [41,42].
- Proposed symmetric hyperbolic systems were not always the best ones for numerical evolution. People are normally still required to re-formulate them for suitable evolution. Such efforts are seen in the applications of the Einstein-Ricci system [54], the Einstein-Christoffel system [45],
- If we can erase the non-principal part by suitable re-definitions of variables (as in the KST formulation) [46], then we can see the growth of the energy norm, Eq. (28), in the numerical evolution, as theoretically predicted [59, 60]. We then see certain differences in the long-term convergence features between weakly and strongly hyperbolic systems.

Of course, these statements are only for a particular formulation, so we have to be careful not to over-emphasize the results.

D. Remarks

In order to figure out the reasons for the above objections, it is worth stating the following cautions:

(a) Rigorous mathematical proofs of well-posedness of PDE are mostly for simple symmetric or strongly hyperbolic systems. If the matrix components or coefficients depend on dynamical variables (as in all any versions of hyperbolized Einstein equations), almost nothing has been proved for more general situations.

(b) The statement of “stability” in the discussion of well-posedness refers to the bounded growth of the norm, Eq. (28) and does not indicate a decay of the norm in the time evolution.

(c) The discussion of hyperbolicity only uses the characteristic part of the evolution equations and ignores the rest.

We think the origin of confusion in the community results from over-expectation for the above issues. Mostly, point (c) is the biggest problem. The above numerical claims based on the Ashtekar [58,61] and the Frittelli-Reula [57] formulations were mostly due to the contribution (or interposition) of non-principal parts in the evolution. Regarding this issue, the KST formulation finally opens the door. KST’s “kinematic” parameters enable us to reduce the non-principal part, so numerical experiments are hopefully expected to represent predicted evolution features from PDE theories. At this moment, the agreement between numerical behavior and theoretical prediction is not yet perfect, but is close [59].

If further studies reveal direct correspondences between theories and numerical results, then the direction of hyperbolization will remain as the essential approach in numerical relativity and the related IBVP research [34, 62–65] will become a main research subject in the future. Meanwhile, it would be useful if we had an alternative procedure to predict stability, including the effects of the non-principal parts of the equations. Our proposal of an adjusted system in the next subsection may be one.

4. Strategy 3: Asymptotically constrained systems

The third strategy is to construct a robust system against the violation of constraints, such that the constraint surface is an attractor (Figure 5). The idea was first proposed as “λ-system” by Brodbeck et al. [66] and was then developed in more general situations as “adjusted system” by the authors [61].

A. The “λ-system”

Brodbeck et al. [66] proposed a system which had additional variables λ that obeyed artificial dissipative equations. The variable λ is supposed to indicate the violation of constraints and the target of the system is to get λ = 0 as its attractor.
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Since the total system is designed to have symmetric hyperbolicity, the evolution is supposed to be unique. Brodbeck et al. showed analytically that such a decay of λ’s can be seen for sufficiently small λ(> 0) with a choice of appropriate combinations of α’s and β’s.

Brodbeck et al. presented a set of equations based on the Frittelli-Reula’s symmetric hyperbolic formulation [43]. The version of Ashtekar’s variables was presented by the authors [67] for controlling the constraints or reality conditions or both. The numerical tests of both the Maxwell-λ-system and the Ashtekar-λ-system were performed [61] and were confirmed to work as expected. The λ-system version of the general-covariant Z4 system [48] is also presented [68]. Pretorius [2] applied this “constraint-damping” idea in his harmonic system to perform his binary black-hole merger simulations.

Although it is questionable whether the recovered solution is a true evolution or not [69], we think the idea is quite attractive. To enforce the decay of errors in its initial perturbative stage seems the key to the next improvements, which are also developed in the next section on “adjusted systems.”

However, there is a high price to pay for constructing a λ-system. The λ-system cannot be introduced generally because (i) the construction of the λ-system requires the original evolution equations to have a symmetric hyperbolic form, which is quite restrictive for the Einstein equations, (ii) the final system requires many additional variables and we also need to evaluate all the constraint equations at every time step, which is a hard task in computation and (iii) it is not clear that the λ-system is robust enough for non-linear violation of constraints or that λ-system can control constraints that do not have any spatial differential terms.

B. The “adjusted system”

Next, we propose an alternative system, which also tries to control the violation of the constraint equations actively, which we named the “adjusted system.” We think that this system is more practical and robust than the previous λ-system. The essentials are summarized as follows:

The adjusted system (procedures):

1. Prepare a set of evolution equations

\[ \partial_t u = J \partial_t u + K. \]  

2. Add constraints in the right-hand-side

\[ \partial_t u = J \partial_t u + K + \kappa C. \]

3. Choose the coefficient (or Lagrange multiplier) \( \kappa \) so as to make the eigenvalues of the homogenized
adjusted $\partial_t C$ equations negative real values or pure imaginary values

$$\partial_t C = D\partial_t C + EC \tag{36}$$
$$\partial_t C = D\partial_t C + EC + F\partial_t C + GC \,. \tag{37}$$

The process of adjusting equations is a common technique in other re-formulating efforts, as we reviewed. However, we try to employ the evaluation process of constraint amplification factors as an alternative guideline to hyperbolization of the system. We will explain these issues in the next section.

\section{A Unified Treatment: Adjusted System}

This section is devoted to present our idea of an "asymptotically constrained system." The original references can be found in Refs. [61], [70], [71] and [30].

\subsection{1. Procedures: Constraint Propagation Equations and Proposals}

Suppose we have a set of dynamical variables $u^a(x^i,t)$ and their evolution equations

$$\partial_t u^a = f(u^a, \partial_i u^a, \cdots), \tag{38}$$

and the (first class) constraints

$$C^\alpha(u^a, \partial_i u^a, \cdots) \approx 0. \tag{39}$$

Note that we do not require that Eq. (38) form a first-order hyperbolic form. We propose to investigate the evolution equation of $C^\alpha$ (constraint propagation),

$$\partial_t C^\alpha = g(C^\alpha, \partial_i C^\alpha, \cdots), \tag{40}$$

for predicting the violation behavior of the constraints in time evolution. We do not mean to integrate Eq. (40) numerically together with the original evolution equations, Eq. (38), but mean to evaluate them analytically in advance in order to re-formulate Eq. (38).

There may be two major analyses of Eq. (40): (a) the hyperbolicity of Eq. (40) when Eq. (40) is a first-order system and (b) the eigenvalue analysis of the whole RHS in Eq. (40) after a suitable homogenization. As we mentioned in Section II.3.D., one of the problems in the hyperbolic analysis is that it only discusses the principal part of the system. Thus, we prefer to proceed down the road (b).

\textbf{Constraint Amplification Factors (CAFs):}

We propose to homogenize Eq. (40) by using a Fourier transformation, e.g.,

$$\partial_t \hat{C}^\alpha = \hat{g}(\hat{C}^\alpha) = M^{\alpha\beta} \hat{C}^\beta,$$

where $C(x,t)^\rho = \int \hat{C}(k,t)^\rho \exp(ik \cdot x) d^3k$, \tag{41}

and then to analyze the set of eigenvalues, say $\Lambda$’s, of the coefficient matrix $M^{\alpha\beta}$ in Eq. (41). We call the $\Lambda$’s the constraint amplification factors (CAFs) of Eq. (40).

The CAFs predict the evolutions of the constraint violations. We, therefore, can discuss the “distance” to the constraint surface by using the “norm” or “compactness” of the constraint violations (although we do not have exact definitions of these “...” words).

The next conjecture seems to be quite useful to predict the evolution features of the constraints:

\textbf{Conjecture on CAFs}

(A) If CAF has a negative real-part (the constraints are forced to be diminished), then we see a more stable evolution than a system which has positive CAF.

(B) If CAF has a non-zero imaginary-part (the constraints are propagating away), then we see a more stable evolution than a system which has zero CAF.

We found that the system became more stable when more $\Lambda$’s satisfied the above criteria. (The first observations were in the Maxwell and Ashtekar formulations [58,61].) Actually, supporting mathematical proofs are available when we classify the fate of the constraint propagations as follows.

\textbf{Classification of Constraint Propagations:}

If we assume that avoiding the divergence of the constraint norm is related to the numerical stability, the next classifications would be useful:

(C1) \textbf{Asymptotically constrained:} All the constraints decay and converge to zero. This case can be obtained if and only if all the real parts of the CAFs are negative.

(C2) \textbf{Asymptotically bounded:} All the constraints are bounded at a certain value. (This includes the above asymptotically constrained case.) This case can be obtained if and only if (a) all the real parts of CAFs are not positive and the constraint propagation matrix $M^{\alpha\beta}$ is diagonalizable, or (b) all the real parts of the CAFs are not positive and the real part of the degenerated the CAFs is not zero.

(C3) \textbf{Diverge:} At least one constraint will diverge.
Q1: Is there a CAF whose real part is positive?

\[ \text{NO} / \text{YES} \]

Diverge

Q2: Are all the real parts of CAFs negative?

\[ \text{NO} / \text{YES} \]

Asymptotically Constrained

Q3: Is the constraint propagation matrix diagonalizable?

\[ \text{NO} / \text{YES} \]

Asymptotically Bounded

Q4: Is a real part of the degenerated CAFs zero?

\[ \text{YES} / \text{NO} \]

Asymptotically Bounded

Q5: Is the associated Jordan matrix diagonal?

\[ \text{NO} / \text{YES} \]

Asymptotically Bounded

Fig. 6. Flowchart to classify the constraint propagations.

The details are shown in Ref. [72]. A practical procedure for this classification is drawn in Figure 6.

The above features of the constraint propagation, Eq. (40), will differ when we modify the original evolution equations. Suppose we add (adjust) the evolution equations by using the constraints

\[
\partial_t u^a = f(u^a, \partial_t u^a, \cdots) + F(u^a, \partial_t u^a, \cdots); \quad (42)
\]

then, Eq. (40) will also be modified as

\[
\partial_t C^a = g(C^a, \partial_t C^a, \cdots) + G(C^a, \partial_t C^a, \cdots). \quad (43)
\]

Therefore, the problem is how to adjust the evolution equations so that their constraint propagations satisfy the above criteria as much as possible.

2. Applications 1: Adjusted ADM Formulations

A. Adjusted ADM equations

Generally, we can write the adjustment terms to Eqs. (6) and (7) using Eqs. (8) and (9) with the following combinations (using up to the first derivatives of constraints for simplicity):

The adjusted ADM formulation [71]:

Modify the evolution equations \( (\gamma_{ij}, K_{ij}) \) by using constraints \( H \) and \( M_i \), i.e.,

\[
\partial_t \gamma_{ij} = (6) + P_{ij} H + Q_{ij} M_k + p_{ij} (\nabla_k H) + q_{ij} (\nabla_k M_l), \quad (44)
\]

\[
\partial_t K_{ij} = (7) + R_{ij} H + S_{ij} M_k + r_{ij} (\nabla_k H) + s_{ij} (\nabla_k M_l), \quad (45)
\]

where \( P, Q, R, S \) and \( p, q, r, s \) are multipliers. According to this adjustment, the constraint propagation equations are also modified as

\[
\partial_t H = (10) + \text{additional terms}, \quad (46)
\]

\[
\partial_t M_i = (11) + \text{additional terms}. \quad (47)
\]

We show two examples of adjustments here. Several others are shown in Table 3 of Ref. [71].

1. The standard ADM vs. original ADM

The first comparison is to show the differences between the standard ADM [19] and the original ADM system [11] (see Section II.1). In the notation of Eqs. (44) and (45), the adjustment

\[
R_{ij} = \kappa_F \alpha \gamma_{ij}, \quad (48)
\]

(and set the other multipliers zero) will distinguish the two, where \( \kappa_F \) is a constant. Here \( \kappa_F = 0 \) corresponds to the standard ADM (no adjustment) and \( \kappa_F = -1/4 \) corresponds to the original ADM (without any adjustment to the canonical formulation by ADM). As one can check by using Eqs. (46) and (47), adding the \( R_{ij} \) term keeps the constraint propagation in a first-order form. Frittelli [73] (see also Ref. [70]) pointed out that the hyperbolicity of the constraint propagation equations is better in the standard ADM system. This stability feature is also confirmed numerically and we set our CAF conjecture so as to satisfy this difference.

2. Detweiler type

Detweiler [74] found that with a particular combination, the evolution of the energy norm of the constraints, \( H^2 + M^2 \), can be negative definite when we apply the maximal slicing condition, \( K = 0 \). His adjustment can be written in our notation in Eqs. (44) and (45) as

\[
P_{ij} = -\kappa_L \alpha^3 \gamma_{ij}, \quad (49)
\]

\[
R_{ij} = \kappa_L \alpha^3 (K_{ij} - (1/3)K \gamma_{ij}), \quad (50)
\]

\[
S_{ij} = \kappa_L \alpha^3 [3(\partial_t(\alpha))\delta^{ij} - (\partial(\alpha))\gamma_{ij} \kappa_l^k], \quad (51)
\]

\[
s_{ij} = \kappa_L \alpha^3 [\delta^{ij} \delta_j^k - (1/3)\gamma_{ij} \kappa_l^k], \quad (52)
\]

and everything else is zero, where \( \kappa_L \) is a multiplier. Detweiler’s adjustment, Eqs. (49)-(52), does not put a constraint propagation equation to a first-order form, so we cannot discuss hyperbolcity or the characteristic speed of the constraints. From a perturbation analysis on the Minkowski and Schwarzschild space-time, we confirmed that Detweiler’s system provides better accuracy than the standard ADM, but only for small positive \( \kappa_L \).

We made various predictions how additional adjusted terms will change the constraint propagation [70, 71].
Fig. 7. Demonstration of numerical evolutions between adjusted ADM systems: especially the standard ADM system and Detweiler’s modified ADM system. The L2 norm of the constraints $H^{ADM}$ is plotted as a function of time. The model is the propagation of a Teukolsky wave in a periodical 3-dimensional box. $k$ is the parameter in Detweiler’s adjustment $|k_L|$ in Eq. (49)-(52), with fixed-$k$ cases (left panel) and with fixed-and-turnoff-$k$ cases (right panel). We see that the life-time of the simulation becomes four-times longer than that of the standard ADM by tuning the parameter $k$.

In that process, we applied the CAF analysis for Schwarzschild spacetime and found when and where the negative real or non-zero imaginary eigenvalues of the homogenized constraint propagation matrix appear and how they depend on the choice of coordinate system and adjustments. We found that there was a constraint-violating mode near the horizon for the standard ADM formulation and that the constraint-violating mode could be suppressed by adjusting equations and by choosing an appropriate gauge conditions.

**B. Numerical demonstrations and remarks**

Systematic numerical comparisons are in progress and we show two sample plots here. Figure 7 is the case of a Teukolsky wave [75] propagating under a 3-dimensional periodic boundary condition. Both the standard ADM system and the Detweiler system [one of the adjusted ADM systems with adjustments Eqs. (49)-(52)] are compared with the same numerical parameters. Plots are the L2 norm of the Hamiltonian constraint $H^{ADM}$, i.e., the violation of constraints and we see the life-time of the standard ADM evolution ends at $t = 200$. However, if we chose a particular value of $k_L$ [multiplier in Eqs. (49)-(52)], we observe that violation of constraints is reduced compared to the standard ADM case and that the simulation can continue longer than that (left panel). If we further tuned $k_L$, say turn-off to $k_L = 0$ when the total L2 norm of $H^{ADM}$ is small, then we can see that the constraint violation is somewhat maintained at a small level, and a more long-term stable simulation is available (right panel).

During the comparisons of adjustments, we found that it is necessary to create a time asymmetric structure of the evolution equations in order to force the evolution onto the constraint surface. There are an infinite number of ways to adjust the equations, but we found that if we followed the next guideline, then such an adjustment would give us a time-asymmetric evolution.

*Trick to obtain asymptotically constrained system:* Break the time reversal symmetry (TRS) of the evolution equation.

1. Evaluate the parity of the evolution equation.
   By reversing the time ($\partial_t \rightarrow -\partial_t$), there are variables that change their signatures (parity $-$) [e.g., $K_{ij}, \partial_t \gamma_{ij}, M_i, \cdots$], while not (parity $+$) [e.g., $g_{ij}, \partial_t K_{ij}, H, \cdots$].

2. Add adjustments that have different parities of that equation.
   For example, for the parity $-$ equation $\partial_t \gamma_{ij}$, add a parity $+$ adjustment $\kappa H$.

One of our criteria, the negative real CAFs, requires breaking the time-symmetric features of the original evolution equations. Such CAFs are obtained by adjusting the terms that break the TRS of the evolution equations and this is available even for the standard ADM system.

**3. Applications 2: Adjusted BSSN formulations**
A. Constraint propagation analysis of the BSSN equations

In order to understand the stability property of the BSSN system, we studied the structure of the evolution equations, Eqs. (17)-(21), in detail, especially how the modifications using the constraints, Eqs. (22)-(26), affect the stability [30]. We investigated the signature of the eigenvalues of the constraint propagation equations and showed that the standard BSSN dynamical equations were balanced from the viewpoint of constrained propagations, including a clarification of the effect of the replacement by using the momentum constraint equation, which was reported by Alcubierre et al. [24].

Moreover, we predicted that several combinations of modifications had a constraint-damping nature and named them the adjusted BSSN systems. Several adjusted BSSN systems are proposed in Table II of Ref. [30].

Yo et al. [31] immediately applied one of our proposals to their simulations of a stationary rotating black hole and reported that one adjustment contributed to maintaining their evolution of the Kerr black hole ($J/M$ up to 0.9$M$) for a long time ($t \sim 6000M$). Their results also indicate that the evolved solution is closer to the exact one, that is, the constrained surface.

Now, let us make clear some current technical tips listed in Section II. 2. B. by using a constraint propagation analysis.

tip-1 The trace-out $A_{ij}$ technique can be explained that the violation of the $A$-constraint, Eq. (25), affects all other constraint violations. (See the full set of constraint propagation equations in the Appendix of Ref. [30].)

tip-2 The replacement of $\bar{\Gamma}^i$ enables to maintain the $G$-constraint, Eq. (24), that delays the violation of $H^{BSSN}$ and $M^{BSSN}_{ij}$. (Again, the statement comes from the full set of constraint propagation equations.)

B. Numerical demonstrations

We recently presented our numerical comparisons of the three kinds of adjusted BSSN formulation [76]. We performed the three testbeds: gauge-wave, linear wave and Gowdy-wave tests, proposed by the Mexico workshop [77] on the formulation problem of the Einstein equations. We observed that the signature of the proposed Lagrange multipliers were always right and that the adjustments improved the convergence and the stability of the simulations. When the original BSSN system already shows satisfactory good evolutions (e.g., linear wave test), the adjusted versions also coincide with those evolutions while in some cases (e.g., gauge-wave or Gowdy-wave tests), the simulations using the adjusted systems last 10 times as long as those using the original BSSN equations.

Figure 8 show a comparison between the (plain) BSSN system and the adjusted BSSN system in the $\bar{A}$-equation by using the momentum constraint

$$\partial_t \bar{A}_{ij} = \partial_t^{\bar{B}} \bar{A}_{ij} + \kappa_A \delta_{ij} \bar{D}_i \bar{M}_j,$$

where $\kappa_A$ is predicted (from the eigenvalue analysis) to be positive in order to damp the constraint violations. The testbed is a one-dimensional gauge-wave, the trivial Minkowski space-time, but sliced with the time-dependent 3-metric. The poor performance of the plain BSSN system for this test has been already reported [78] and one remedy is to apply a 4th-order finite differencing scheme [79]. The plots show that our adjusted system...
also improved the life-time of the plain BSSN simulation by at least 10 times with better convergence.

IV. OUTLOOK

1. What we have achieved

We reviewed recent efforts to the formulation problem of numerical relativity, the problem to find a robust system against constraint violations. We categorized the approaches into

(0) The standard ADM formulation (Section II.1),
(1) The BSSN formulation (Section II.2),
(2) Hyperbolic formulations (Section II.3) and
(3) Asymptotically constrained formulations (Section II.4).

Most numerical relativity groups now use the BSSN set of equations, which are obtained empirically. A dramatic announcement of the success of binary black-hole simulations has caused the community to follow that recipe. Actually, we do not yet completely understand why the current set of BSSN equations, together with particular combinations of gauge conditions, works well. Several explanations are applied based on the hyperbolic formulation scheme, but as we viewed, they are not yet satisfactory.

Our approach, on the other hand, tries to construct an evolution system that has its constraint surface as an attractor. Our unified view is to understand the evolution system by evaluating its constraint propagation. Especially, we propose to analyze the constraint amplification factors that are the eigenvalues of the homogenized constraint propagation equations. We analyzed the system based on our conjecture whether the constraint amplification factors suggest a constraint to decay/propagate or not. We concluded that

- The constraint propagation features become different by simply adding constraint terms to the original evolution equations (we call this an adjustment of the evolution equations).
- There is a constraint-violating mode in the standard ADM evolution system when we apply it to a single non-rotating black hole space-time and its growth rate is larger near the black-hole horizon.
- Such a constraint-violating mode can be killed if we adjust the evolution equations with a particular modification using constraint terms. An effective guideline is to adjust terms as they break the time-reversal symmetry of the equations.
- Our expectations are borne out in simple numerical experiments using the Maxwell, the Ashtekar and the ADM systems. However, the modifications are not yet perfect to prevent non-linear growth of the constraint violation.
- We understand why the BSSN formulation works better than the ADM one in a limited case (perturbation analysis in the flat background); further, we propose modified evolution equations along the lines of our previous procedure. Some of these proposed adjusted systems are numerically confirmed to work better than the standard BSSN system.

The common key to the problem is how to adjust the evolution equations with constraints. Any adjusted systems are mathematically equivalent if the constraints are completely satisfied, but this is not the case for numerical simulations. Replacing terms with constraints is one of the normal steps when people re-formulate equations in a hyperbolic form.

In summary, let me answer the following three questions:

- What is the guiding principle for selecting the evolution equations for simulations in GR?
  - The key is to analyze the constraint propagation equation of the system.
- Why do many groups use the BSSN equations?
  - Because people just rush, not to be behind others.
- Is there an alternative formulation better than the BSSN?
  - Yes, there is, but we do not know which is the best one yet.

2. Future directions

If we say the final goal of this project is to find a robust evolution system against violation of constraints, then the recipe should be a combination of (a) formulations of the evolution equations, (b) choice of gauge conditions, (c) treatment of boundary conditions and (d) numerical integration methods. We are now in the stages of solving these mixed puzzles. Recent attention to higher dimensional space-time studies is waiting for numerical research, but it is known that the formulation problem also exists in higher-dimensional cases [80].

We have written this review from the viewpoint that general relativity is a constrained dynamical system. This is not a proper problem in general relativity, but it is in many physical systems, such as electrodynamics, magnetohydrodynamics, molecular dynamics and mechanical dynamics. Therefore, sharing and discussing thoughts between different fields will definitely accelerate the progress. The ideal algorithm to solve all the problems may not exist, but the author believes that our
final numerical recipe is somewhat an automatic system and hopes that numerical relativity turns to be an easy toolkit for everyone in the near future.

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