Constraint damping of the conformal and covariant formulation of the Z4 system in simulations of binary neutron stars

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Following previous work in vacuum spacetimes, we investigate the constraint-damping properties in the presence of matter of the recently developed traceless, conformal and covariant Z4 (CCZ4) formulation of the Einstein equations. First, we evolve an isolated neutron star with an ideal gas equation of state and subject to a constraint-violating perturbation. We compare the evolution of the constraints using the CCZ4 and Baumgarte-Shibata-Nakamura-Oohara-Kojima (BSSNOK) systems. Second, we study the collapse of an unstable spherical star to a black hole. Finally, we evolve binary neutron star systems over several orbits until the merger, the formation of a black hole, and up to the ringdown. We show that the CCZ4 formulation is stable in the presence of matter and that the constraint violations are 1 or more orders of magnitude smaller than for the BSSNOK formulation. Furthermore, by comparing the CCZ4 and the BSSNOK formulations also for neutron star binaries with large initial constraint violations, we investigate their influence on the errors on physical quantities. We also give a new, simple and robust prescription for the damping parameter that removes the instabilities found when using the fully covariant version of CCZ4 in the evolution of black holes. Overall, we find that at essentially the same computational costs the CCZ4 formulation provides solutions that are stable and with a considerably smaller violation of the Hamiltonian constraint than the BSSNOK formulation. We also find that the performance of the CCZ4 formulation is very similar to another conformal and traceless, but noncovariant formulation of the Z4 system, i.e., the Z4c formulation.

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I. INTRODUCTION

Recent developments in numerical reliability allow for the simulation of binary compact objects, e.g., binary neutron star (NS) systems, which are among the strongest sources of gravitational waves. Given that less than one decade ago, even the vacuum binary black hole (BH) problem was still a challenge for numerical evolutions of the Einstein equations, the progress is indeed remarkable. Part of this rapid progress is surely due to a better understanding of the mathematical properties of the different formulations of the Einstein equations and the choice of suitable gauge conditions. The most widely used formulation of the Einstein equations in three-dimensional numerical simulations is given by a conformal and traceless formulation of the ADM (Arnowitt-Deser-Misner) 3+1 decomposition of the Einstein equations [1,2], and is also known as the BSSNOK (or BSSN) formulation [3-5].

Another conformal and traceless formulation, i.e., the CCZ4 formulation, was introduced recently in Ref. [6] (hereafter paper I), where we discussed in detail its structure and properties. The CCZ4 formulation shares some important properties with the BSSNOK formulation. It allows for stable evolutions in conjunction with robust and singularity-avoiding gauges, thus eliminating the need for excision techniques, and with simple Sommerfeld radiative boundary conditions. The main advantage of the CCZ4 formulation over the BSSNOK formulation is its ability to dynamically evolve the constraints equations and to couple them with a constraint-damping scheme that leads to a rapid suppression of the violations that are inevitably produced in numerical simulations.

In paper I, we validated the properties of the CCZ4 system in evolutions of single and binary BH systems. The constraint-propagating and damping properties of the system turned out to be very useful in reducing the violations produced in long-term simulations and led to constraint violations that were, on average, 1 order of magnitude smaller than those with the BSSNOK system. In this work, we investigate the behavior of the CCZ4 system also in evolutions of nonvacuum spacetimes, in particular those of single and binary NSs. In paper I, the simulations were performed with both a multipatch coordinate system, where the spherical outer boundary was causally disconnected, and Cartesian grids plus radiative boundary conditions. In the latter system, we noticed reflections from the outer boundary which led to an increase in the values of the constraints. However, these violations were rapidly damped, and there was no sign of instabilities produced in relation with the outer boundary. In this work, we focus on the latter case, which is used more often in simulations of neutron star mergers.

We recall that the CCZ4 system contains three constant parameters, one of which ($k_3$, see below) determines if the system is actually covariant or not (throughout this paper we refer to both versions as CCZ4). It is obviously advantageous if the propagation equations for the constraints are covariant, since it allows one to generalize results found in a particular coordinate system. For noncovariant formulations, on the other hand, the behavior of the constraint evolution could in principle be radically altered when going, for example, from Cartesian to spherical coordinates. This is relevant in practice when comparing one-dimensional and three-dimensional evolutions or when using multipatch coordinate systems. While both covariant and noncovariant formulations were studied in paper I, we also found there that exponentially growing modes appear for the fully covariant system. An important point of this paper is the exploration of the behavior of the covariant
and noncovariant versions of the CCZ4 system in spacetimes containing matter. We will show that the aforementioned instabilities occur only when a BH is present in the spacetime, while simulations of NSs do not show such instabilities. Furthermore, we will demonstrate that even when a BH appears in the solution, e.g., in the collapse of a NS, or after the merger of two NSs, a modification of the damping terms in the fully covariant CCZ4 system results in stable evolutions. Finally, we will also confirm that in all comparisons between the covariant and the noncovariant versions of the CCZ4 system, the differences between the results are very small.

A different conformal version of the noncovariant Z4 system has been presented in Refs. [7–11]. This system, called Z4c, removes sources terms in order to bring the evolution equations into a form which is closer to the BSSNOK system. Recent numerical results obtained with Z4c in three-dimensional simulations of compact objects [11] report a reduction in the Hamiltonian constraint violation between 1 and 3 orders of magnitude with respect to BSSNOK for nonvacuum spacetimes, and between 1 and 2 orders of magnitude for black hole spacetimes. Performing a similar comparison of the Z4c and BSSNOK systems, we could measure a reduction of constraint violations of only 1 or 2 orders of magnitude, probably because we lack the improvement associated with Z4c, that comes from the use of constraint-preserving boundary conditions of the type described in Ref. [8]. The direct comparison between the CCZ4 and Z4c systems shows that the CCZ4 leads to similarly low constraint violations and allows long-term stable evolution when coupled with standard radiative boundary conditions. Analytically, there are no features intrinsic to the Z4c system which suggest improvement over CCZ4.

The plan of the paper is as follows: Section [II] presents an overview of the CCZ4 system of the Einstein equations coupled with the hydrodynamic equations, as well as the numerical infrastructure of our simulations. Section [III] is dedicated to numerical results obtained with the CCZ4 system in evolutions of a stable, isolated NS, of the collapse of an unstable NS to a BH, and of binary NS systems, both with constraint-satisfying and constraint-violating initial data. In the first four subsections, we compare results obtained with the BSSN and CCZ4 formulations of the Einstein equations, while the last two subsections are dedicated to a comparison with the Z4c system and between the fully covariant and the noncovariant versions of the CCZ4 system. We conclude with the summary and discussions in Sec. [IV].

Throughout this paper, we use a metric signature of \((- , + , + , +)\) and units in which \(c = G = M_\odot = 1\), unless noted otherwise. Greek indices are taken to run from 0 to 3, Latin indices from 1 to 3, and we adopt the standard convention for summation over repeated indices.

### II. FORMULATION AND NUMERICAL METHODS

#### A. The CCZ4 system

The CCZ4 system is a conformal and covariant formulation of the Einstein equations. It is based on a conformal transformation of the Z4 system (see paper I), which converts the original Hamiltonian and momentum ADM constraints into evolution equations for a four-vector \(Z_\mu\). This amounts to introducing two additional evolution variables, namely the projection \(\Theta\) along the normal direction of the four-vector \(Z_\mu\) and its spatial component \(Z_i\). The system can be supplemented with damping terms [12], which ensure exponential damping of the constraint violations in numerical evolutions.

The steps required to convert the original Z4 system into a conformal version were presented in our previous paper I. For completeness, we summarize here the main ideas behind the Z4 formulation and point to Refs. [13–14] for more details about its properties. The CCZ4 system is given by the following set of evolution equations:

\[
\begin{align*}
\partial_t \gamma_{ij} &= -2\alpha A^i_j + 2\gamma_{kh} \partial_j \beta_k - \frac{2}{3} \tilde{\gamma}_{ij} \partial_k \beta_k + \beta_k \partial_k \tilde{\gamma}_{ij}, \\
\partial_t A_i &= \phi^2 \left[ -\nabla_i \nabla_j \alpha + \alpha (R_{ij} + \nabla_i Z_j + \nabla_j Z_i - 8\pi S_{ij}) \right]_{\text{TP}} + \alpha A_j (K - 2\Theta) \\
&- 2\alpha \tilde{A}_k A^j_i + 2\tilde{A}_k (\partial_j \beta_k) - \frac{2}{3} \tilde{A}_{ij} \partial_k \beta_k + \beta_k \partial_k \tilde{A}_{ij} , \\
\partial_t \phi &= \frac{1}{3} \alpha \phi K - \frac{1}{3} \phi \partial_i \beta^i + \beta_i \partial_i \phi , \\
\partial_t K &= -\nabla^i \nabla_i \alpha + \alpha (R + 2\nabla_i Z^i - 2K - 2\Theta K) + \beta_j \partial_j K - 3\alpha \kappa_1 (1 + \kappa_2) \Theta + 4\pi \alpha (S - 3\tau) , \\
\partial_t \Theta &= \frac{1}{2} \left[ R + 2\nabla_i Z^i - \tilde{A}_{ij} A^{ij} + \frac{2}{3} K^2 ( -2\Theta K) \right] - Z^i \partial_i \alpha + \beta_k \partial_k \Theta - \alpha \kappa_1 (2 + \kappa_2) \Theta - 8\pi \alpha K , \\
\partial_t \tilde{\Gamma}^i = 2\alpha \left[ \tilde{\Gamma}_k^i \tilde{A}^k - 3\tilde{A}^i \partial \phi \right] - \frac{2}{3} \tilde{\gamma}_{ij} \partial_j \tilde{\Gamma}^i + 2\tilde{\gamma}^{kj} \left( \alpha \partial_k \Theta - \Theta \partial_k \alpha - \frac{2}{3} \alpha K \tilde{Z}_k \right) - 2\tilde{A}^j \partial_j \alpha \\
&+ \tilde{\gamma}^{kj} \partial_k \tilde{\Gamma}^j + \frac{1}{3} \tilde{\gamma}_{ij} \partial_k \beta_i + \frac{2}{3} \tilde{\gamma}^{kj} \partial_k \beta^i - \tilde{\Gamma}^i \partial_k \beta_k + 2\kappa_3 \left( \frac{2}{3} \tilde{\gamma}^{kj} Z_j \partial_k \beta^i - \tilde{\gamma}^{jk} Z_j \partial_k \beta^i \right) \\
&+ \beta_k \partial_k \tilde{\Gamma}^i - 2\alpha \kappa_1 \tilde{\gamma}^{ij} Z_j - 16\pi \alpha \tilde{\gamma}^{ij} S_j ,
\end{align*}
\]
where \( \tilde{\gamma}_{ij} = \phi^2 \gamma_{ij} \) is the conformal metric with unit determinant \( \phi = (\det(\gamma_{ij}))^{1/6} \), while the extrinsic curvature \( K_{ij} \) is represented by its trace \( K \equiv K_{ij} \gamma^{ij} \) and its trace-free components

\[
\tilde{A}_{ij} = \phi^2 (K_{ij} - \frac{1}{3} K \gamma_{ij}).
\]

The following definitions apply for matter-related quantities

\[
\tau \equiv n_\mu n_\nu T^{\mu\nu}, \quad S_i \equiv n_\mu T_i^\mu, \quad S_{ij} \equiv T_{ij},
\]

and \( \Theta \) is the projection of the Z4 four-vector along the normal direction, \( \Theta \equiv n_\mu Z^\mu = \alpha Z^0 \). We note that we here follow the definition of the normal four-vector suggested in Ref. \([13]\), i.e., \( n_\mu = (\alpha, 0) \) and \( n^\mu = (-1/\alpha, \beta^i/\alpha) \), which is different from the more traditional one in which \( n_\mu = (-\alpha, 0) \) and \( n^\mu = (1/\alpha, -\beta^i/\alpha) \). These different definitions do not affect the form of the CCZ4 equations.

The evolution variable \( Z_j \) of the Z4 formulation is now included in the \( \Gamma^i \) variable of the CCZ4 formulation

\[
\tilde{\Gamma}^i \equiv \hat{\Gamma}^i + 2\tilde{\gamma}^{ij} Z_j,
\]

where

\[
\hat{\Gamma}^i \equiv \tilde{\gamma}^{jk} \tilde{\Gamma}_j^i = \tilde{\gamma}^{ij} \tilde{\gamma}^{kl} \partial_k \tilde{\gamma}_{jk}.
\]

The numerical simulations presented in this paper use as gauge conditions the “1 + log” slicing

\[
\partial_t \alpha = -2\alpha (K - 2\Theta) + \beta^k \partial_k \alpha,
\]

and the gamma-driver shift condition

\[
\partial_t \beta^i = f B^i + \beta^k \partial_k \beta^i,
\]

\[
\partial_t B^i = \partial_t \hat{\Gamma}^i - \beta^k \partial_k \hat{\Gamma}^i + \beta^k \partial_k B^i - \eta B^i,
\]

where the gauge parameter \( f \) is set to 3/4. We adopt the “constrained approach” from paper I in order to enforce the constraints of the conformal formulation (trace cleaning).

We also compute the constraint violations introduced by the numerical evolution in the ADM constraints:

\[
H = R - K_{ij} K^{ij} + K^2 - 16\pi \tau,
\]

\[
M_i = \gamma^{kl} (\partial_l K_{ij} - \partial_l K_{jl} - \Gamma^m_{jl} K_{mi} + \Gamma^m_{jl} K_{mi}) - 8\pi S_i.
\]

For both the BSSNOK and the CCZ4 systems, we compute the ADM quantities from the evolved variables of the two systems.

The three-dimensional Ricci tensor \( R_{ij} \) is split into a part \( \tilde{R}_{ij} \) containing conformal terms and another one, \( \hat{R}_{ij} \), containing space derivatives of the conformal metric, defined as

\[
\tilde{R}_{ij} = \frac{1}{2} \tilde{\gamma}^{lm} \partial_l \partial_m \tilde{\gamma}_{ij} + \tilde{\gamma}_{k(i} \tilde{\partial}_{j)} \tilde{\Gamma}^k + \tilde{\Gamma}^{ik} \tilde{\Gamma}_{(ij)k} + \frac{1}{2} \tilde{\gamma}^{lm} \left[ 2\tilde{\Gamma}_{l(i} \tilde{\Gamma}_{j)km} + \tilde{\Gamma}_{l(i} \tilde{\Gamma}^k_{jm} \right],
\]

\[
\hat{R}_{ij} = \frac{1}{\phi^2} \left[ \phi \left( \tilde{\nabla}_i \tilde{\nabla}_j \phi + \tilde{\gamma}_{ij} \tilde{\nabla}_k \phi \right) - 2\tilde{\gamma}_{ij} \tilde{\nabla}^k \phi \tilde{\nabla}_k \phi \right].
\]

We recall that the parameters \( \kappa_1 \) and \( \kappa_2 \) control the damping terms and that all the constraint-related modes are damped when \( \kappa_1 > 0 \) and \( \kappa_2 > -1 \) \([12]\). The third coefficient, \( \kappa_3 \), instead affects some quadratic terms in the evolution for \( \Gamma^i \) Eq. \([6]\) and determines the covariance of the corresponding CCZ4 system. In particular, a value of \( \kappa_3 = 1 \) corresponds to full covariance. While \( \kappa_2 \) and \( \kappa_3 \) are dimensionless, \( \kappa_1 \) is the damping timescale, which we report in geometric units with \( M_0 = 1 \).

We also recall that in paper I we performed numerical experiments with the covariance parameter \( \kappa_3 \) and concluded that a choice of \( \kappa_3 = 1 \) and \( \kappa_1 = \text{const.} \) leads to unstable behavior in the context of black hole spacetimes. Even though we could not fully isolate the cause of these numerical instabilities, we found that they are produced by nonlinear couplings with the damping terms, which are important for reducing the violations in the constraints. As a result, all of the tests reported in paper I made use of \( \kappa_3 = 1/2 \), which, for consistency with paper I, is also the value we will use for the majority of the tests discussed here. Two important remarks should, however, be made now, although they will be discussed also later on. First, in the presence of a nonsingular spacetime with matter, a fully covariant formulation (i.e., with \( \kappa_3 = 1 \)) does not show any of the pathologies encountered in paper I with black holes. The pathologies, however, do appear as soon as a black hole is formed. Second, we have devised a new prescription for the damping term \( \kappa_1 \) which couples it to the lapse function and cures these instabilities also when black holes appear in the evolution. As a result, independently of whether we are considering vacuum or nonvacuum spacetimes, our CCZ4 formulation can now always be used in its fully covariant form. A more extended discussion of this point, with the presentation a series of examples, is postponed to Sec. III F.

As mentioned in the Introduction, another noncovariant but conformal formulation of the Z4 system has been proposed recently in Ref. \([11]\), namely the Z4c formulation. The suggestion behind the Z4c formulation is that of introducing the damping features of the Z4 formulation with only minimal changes to the BSSNOK system. As we will comment later on, this strategy is a very reasonable one and leads to results
that are comparable to those of the CCZ4 formulation and whose main drawback is being noncovariant. While this aspect of the formulation may be harmless in practice, it makes it difficult to generalize the properties found in a particular coordinate system, leaving room for unexpected behavior.

Because the CCZ4 and Z4c formulations differ only in non-principal part terms, we have marked the terms that are missing in the Z4c formulation with blue boxes within the set of evolution equations Eqs. [1]-[6]. In addition, the Z4c system evolves the trace of the extrinsic curvature $\hat{K}$ using an evolution equation similar to the BSSNOK one [11] to replace Eq. (4).

\[
\partial_t \hat{K} = -\nabla^i \nabla_i \alpha + \alpha \left( \hat{A}_{ij} \hat{A}^{ij} + \frac{1}{3} (\hat{K} + 2\Theta)^2 \right) + \beta^j \partial_j \hat{K} + \alpha \kappa_1 (1 - \kappa_2) \Theta + 4\pi\alpha (S + \tau)
\]

(18)

to replace Eq. (4). This variable can be translated in CCZ4 terms as

\[
\hat{K} = K^{\text{BSSNOK}} = K - 2\Theta.
\]

B. The relativistic hydrodynamic equations

We evolve the hydrodynamic equations in flux-conservative form as

\[
\partial_t \hat{D} = -\partial_k \left[ w^k D \right],
\]

(20)

\[
\partial_t \hat{\tau} = -\partial_k \left[ w^k \hat{\tau} + \phi^{-3} \alpha \rho w^k \right] + \alpha \hat{S}_{lm} K_{lm} - \hat{S}^k \partial_k \alpha,
\]

(21)

\[
\partial_t \hat{S}_i = -\partial_k \left[ w^k \hat{S}_i + \phi^{-3} \alpha \rho w^k \delta^i_k \right] + \frac{\alpha}{2} \hat{S}_{lm} \partial_l \gamma_{im} + \hat{S}_k \partial_i \beta^k - (\hat{\tau} + \hat{D}) \partial_i \alpha.
\]

(22)

The evolved variables are the conserved energy density $\hat{D}$, the conserved energy density $\hat{\tau}$, and the conserved momentum density $\hat{S}_i$, whose definition is given by

\[
\hat{D} \equiv \phi^{-3} \rho W, \quad \hat{\tau} \equiv \phi^{-3} (\rho h W^2 - p) - \hat{D}, \quad \hat{S}_i \equiv \phi^{-3} \rho h W^2 v_i.
\]

(23, 24, 25)

Above, $\rho$ is the rest mass density, $v^i$ is the 3-velocity, $W$ is the Lorentz factor, $\rho w^i \equiv \alpha \rho w^i - \beta^i$ is the advection speed with respect to the coordinates, $p$ is the pressure, $\epsilon$ is the specific internal energy, and $h = 1 + \epsilon + p/\rho$ is the specific enthalpy. Finally, the projection of the energy-momentum tensor onto the spatial hypersurfaces of the foliation leads to the spatial tensor

\[
\hat{S}_{ij} \equiv \phi^{-3} \left( \rho h W^2 v_i v_j + \gamma_{ij} p \right).
\]

(26)

C. Numerical setup

To evolve the hydrodynamic equations, we rely on an improved version of the Whisky code described in Refs. [15-19], but without making use of the ideal MHD part or of the high-order finite difference operators. The evolution of the spacetime is performed using our CCZ4 implementation within the McLachlan code [20], which is part of the publicly available Einstein Toolkit infrastructure based on the Cactus computational framework. For the time integration we are using the method of lines with an explicit fourth-order Runge-Kutta method. The outer boundary conditions used are the (Sommerfeld) radiative ones provided by the McLachlan code, initially developed and well tested for the BSSNOK system.

We employ adaptive mesh refinement (AMR) for our numerical grid, provided via the Carpet driver [21]. For single-star simulations, we use a fixed grid hierarchy, while for binary NS runs we follow the centers of mass of the stars with moving refined boxes. During the merger, they are replaced by larger nonmoving refinement regions of the same resolution. Shortly after, one more refinement level with doubled resolution is activated to better resolve the black hole.

For the solution of the Einstein equations we use finite-difference spatial differential operators of various orders, although the results presented in this paper have been obtained using fourth-order-accurate schemes. The spatial discretization of the hydrodynamic equations, on the other hand, uses a finite-volume high-resolution shock-capturing scheme adopting the parabolic reconstruction of the piecewise parabolic method (PPM) [22] and the Harten-Lax-van Leer-Einfeldt (HLLE) [23] approximate Riemann solver. In contrast to the original Whisky code, we do not reconstruct the 3-velocities $v^i$, but rather the quantities $Wv^i$ (as done in Ref. [18]). This guarantees that the velocities reconstructed at the cell boundaries stay subluminal even under the extreme conditions which occur at the center of a black hole. Using shock tube tests, we verified that this modification does not affect the treatment of shocks.

Furthermore, we improved the robustness of the conversion algorithm from evolved to primitive variables, allowing a clear distinction between physical and unphysical values. The details of this algorithm have already been described in Ref. [18]. For the current work, the only important aspect of the improvements is the ability to enforce a fine-grained error policy. The standard policy does not allow any unphysical values, with the exception of the internal energy falling below the zero temperature value (zero for the ideal gas equation of state EOS), in which case it is reset to that value. This can happen frequently when evolving cold matter, where the internal energy is exactly at the minimum value allowed by the given EOS. At densities corresponding to the surface region of the star, which is a notorious source of errors in hydrodynamic simulations, we use a more lenient policy, which adjusts unphysical values of the conserved energy and momentum densities to the physically meaningful range at a given density. The same applies to a region around the center of the black hole, which we define as the region in which $\alpha \leq \alpha_c = 0.1$.
and which is always contained within the apparent horizon. In this region we also limit the Lorentz factor to be \( W \leq 3 \). This adjustment, together with the aforementioned modified reconstruction, allows us to evolve a black hole without excision for the spacetime or for the hydrodynamic variables.

Finally, we added an option to smoothly remove all matter from the center of a black hole. We did this to investigate how the presence of matter at the center of the black hole affects the numerical errors in comparison to an evolution of a vacuum black hole. This needs to be addressed separately from the spacetime-matter coupling elsewhere, because, although our gauge is singularity avoiding, the gradients of metric and density close to the center of a BH still become so large that it is always severely under-resolved numerically. To remove the matter, we introduce a term \(-q/\tau_d\) to the rhs of the conserved variables \( q = (D, \tau, S_i) \). The baryon mass then evolves according to \( \dot{M}_b = -M_b/\tau_d \), thus leading to an exponential decay.

In simulations that form a black hole, we detect apparent horizons using the module AHFinderDirect \[24\] from the Einstein toolkit. We compute the mass and spin using the isolated horizon formalism \[25, 26\] implemented in the QuasiLocalMeasures module. Finally, the constraints in Eqs. (16)-(17) are computed using a standard fourth-order finite difference method.

### III. RESULTS

In this section, we investigate the stability of the CCZ4 formulation when coupled to matter and test the convergence properties of the code. Furthermore, we compare the behavior of the constraint violations, first between the CCZ4 and the BSSNOK formulations, then between the CCZ4 and the Z4c formulations, and finally between the covariant and the noncovariant CCZ4 versions.

#### A. Isolated neutron star

For our first comparison, we choose an isolated, spherically symmetric NS. The initial data obey a polytropic EOS, \( i.e., P = K \rho^\Gamma \), with \( \Gamma = 2 \) and \( K = 100 \). During the evolution, we use a matching ideal gas EOS with \( \Gamma = 2 \). The star has a (gravitational) mass of \( M = 1.4 \, M_\odot \) and a circumferential radius of \( R = 14.16 \, \text{km} \). The grid setup can be found in Table I.

In order to add a well-defined initial constraint violation, we perturb the star with an eigenfunction of the \( \ell = 2, m = 0 \) fundamental mode in the Cowling approximation. The amplitude we used corresponds to a radial velocity of 0.017 at the surface. Because a corresponding perturbation in the metric is not introduced, the Hamiltonian and momentum constraints are violated in exactly the same way for CCZ4 and BSSNOK simulations.

When evolved in time, both formulations lead to stable solutions, and the dynamics of the simulations agrees very well between BSSNOK and CCZ4, with a relative difference in the central rest mass density that after 7.1 ms is only \( 3 \times 10^{-4} \). For comparison, the amplitude of the oscillations corresponds to a relative change of 0.015. The constraint violations are shown in Fig. 1. Since the components \( M^i \) of the momentum constraint are very similar, we show the combined norm \( \|M\|_2 \equiv \sqrt{\sum_i (\|M^i\|_2)^2} \). Clearly, the Hamiltonian constraint is damped efficiently by the CCZ4 formulation already after about 1 ms and is about 2 orders of magnitude smaller at the end of the simulation, \( i.e., t \approx 7 \, \text{ms} \). The BSSNOK formulation, on the other hand, exhibits a growth after a short initial decrease. In this setup, the momentum constraints are on average very similar for the CCZ4 and BSSNOK formulations.

Besides investigating the constraints, we also use this setup to test the convergence properties of the code. For this we use three different grid spacings, \( i.e., \Delta x = 443.0, 295.3, 199.5 \, \text{m} \) on the finest level, differing by a factor of 1.5, and evolved up to \( t = 6.5 \, \text{ms} \). For the variables \( \alpha, \rho, \gamma \), we then measure the convergence order as follows: First, we select the time steps that are common to all resolutions. Next, we select the grid points on the finest refinement level which are present for each resolution. Then we compute for each variable and time step the differences between the results for low and medium resolutions, as well as those between the results for medium and high resolutions. Finally, we compute the \( L_1, L_2, \) and \( L_\infty \) norms of those differences over the selected grid points, and compute the time average of the norms. From those values we compute the convergence order \( n \), assuming the errors converge following a power law. We also compute the convergence order obtained at each time, which is shown in Fig. 2. For the lapse function, we find an overall convergence order of \( n = 1.96, 2.07, 2.87 \) for the \( L_1, L_2, \) and \( L_\infty \) norms, respectively, while for \( \gamma \) we

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**FIG. 1:** Comparison of the CCZ4 and BSSNOK formulations in the evolution of a single and perturbed TOV star. The CCZ4 runs use the parameters \( \kappa_1 = 0.02, \kappa_2 = 0 \). Shown are the \( L_2 \) norms of the Hamiltonian (top panel) and the combined momentum (bottom panel) constraint violations, taken over the full computational domain.
obtain \( n = 1.83, 1.98, 2.62 \). For the rest mass density \( \rho \), on
the other hand, we find \( n = 1.45, 1.53, 1.85 \).

The convergence order we would expect from the combined
numerical schemes for spacetime and fluid in regions where
fluid quantities are smooth and no fluid-vacuum boundary is
present is 2. However, the convergence of the hydrodynamic
equations part is reduced near the surface of the star because
of the use of an artificial atmosphere; furthermore, the conver-
gence order also drops to 1 near shocks (although no global
shocks are present in this test) and at local maxima. Because
of these contaminations, the effective convergence order for
the hydrodynamic equations is smaller, around \( n \approx 1.5 \). On
the other hand, the reason why the spacetime variables show
better convergence in the given resolution range is probably
that the spacetime is mainly influenced by the bulk properties
of the matter, which are less affected by the aforementioned
problems. These results are in good agreement with what was
found when analyzing the convergence order of the wave-
forms from binary NSs, which we will discuss in Sec. [HID]
(see also Ref. [27]).

| Simulation (stage) | \( h_0 \) [km] | \( h_f \) [km] | Levels | \( R_n \) [km] | \( R_{\text{stat}} \) [km] | \( R_{\text{BH}} \) [km] | \( M \[M_{\odot}\] | symmetries |
|-------------------|----------------|----------------|--------|---------------|----------------|----------------|----------------|---------|
| Stable TOV        | 1.1814         | 0.2953         | 3 (0)  | (94.5, 47.3, 23.6) | 14.2           | –              | 1.40           | octant |
| Unstable TOV      | 1.4746         | 0.1843         | 4 (0)  | (118.0, 59.0, 29.5, 14.7) | 8.59           | 4.24           | 1.44           | octant |
| BH*               | 1.4746         | 0.1843         | 4 (0)  | (118.0, 59.0, 29.5, 14.7) | –              | 3.41           | 1.44           | octant |
| BH                | 1.4746         | 0.0921         | 5 (0)  | (150.4, 82.6, 36.8, 18.4, 8.1) | –              | 2.36           | 1.00           | octant |
| Binary NS (inspiral) | 9.4510         | 0.2953         | 6 (2)  | (756.1, 354.4, 177.2, 94.5, 32.5, 16.2) | 12.4           | –              | 1.57           | \( z \) and \( \pi \) |
| Binary NS (merger) | 9.4510         | 0.2953         | 6 (0)  | (756.1, 354.4, 177.2, 94.5, 37.8, 21.6) | –              | –              | –              | \( z \) and \( \pi \) |
| Binary NS (collapse) | 9.4510        | 0.1477         | 7 (0)  | (756.1, 354.4, 177.2, 94.5, 37.8, 21.6, 10.8) | –              | 3.60           | 3.20           | \( z \) and \( \pi \) |

TABLE I: Grid setups of our simulations. Here, \( h_0 \) and \( h_f \) denote, respectively, the coarsest and finest grid spacing, \( R_n \) are the radii of each refinement level (in case of levels with moving boxes, the radius of each box), \( R_{\text{stat}} \) is the initial neutron star coordinate radius, \( R_{\text{BH}} \) the coordinate radius of the final BH, if present, and \( M \) is the gravitational mass of the NS or of the BH. Note that the simulation BH* refers to a stationary BH evolved with a numerical domain with extents rescaled so that they match those of the collapsing star.

B. Collapse to a black hole

Our next test consists of a NS on the unstable branch, to
which we apply a small inwards velocity kick in order to trig-
ger a collapse to a black hole. We use the same EOS as for the
stable TOV test in the previous section, but the central density
is \( 5 \times 10^{15} \text{ g \ cm}^{-3} \), the gravitational mass is \( M = 1.44 M_{\odot} \),
and the circumferential radius is \( R = 8.59 \text{ km} \). The velocity
perturbation is simply given by \( \psi' = \psi R / \psi' \), with \( \psi = -0.01 \).
The purpose of this test is not only to compare the constraint
violations between the CCZ4 and the BSSNOK formulations,
but also to show that both formulations lead to a stable evolution
of the black hole when coupled to matter.

We observe that the infalling matter ends up in the cen-
tral numerical cell. The matter then stays there; the relative
change of total baryon mass between \( t = 5 \text{ ms} \) (after the
collapse) and \( 5 \text{ ms} \) is less than \( 10^{-7} \). The profile of the lapse
function, shift vector, density, and metric determinant all ap-
proach stationary values shortly after the BH has formed.
Between \( 1.9 \) and \( 5 \text{ ms} \), the lapse function at the center changes
by less than 3%. There is, however, a numerical instability
in the fluid velocity inside the cell at the center of the BH,
but since we limit the maximum velocity at the center of the
BH as described in Sec. [HIC] this quickly becomes stationary as
well.

The evolution of the constraints is shown in Fig. [3]. For
comparison, we evolved a Schwarzschild BH of the same
mass using the CCZ4 spacetime evolution code without the
fluid part, but with the same grid setup. As shown in Fig. [3]
the constraint violations are very similar to the collapse simu-
lation after the BH has formed. The \( L_2 \) norms excluding the
BH interior agree very well, not only in magnitude but also in
terms of the long-time behavior.

The norms including the BH interior (not shown in the plot)
for vacuum BH and collapse agree very well initially. How-
ever, when the aforementioned instability develops during the
evolution with matter, the norm of the momentum constraint is
in order to exponentially remove the matter over an e-folding timescale $\tau_d = 0.025$ ms. This source term is only active near the center of the BH, which we define for simplicity via the lapse function by the condition $\alpha < 0.007$. The instability at the center of the BH and the corresponding jump in the momentum constraint do not occur anymore when using this method. However, there is no visible change of the norm of the constraint violations outside the BH.

We conclude that the constraint violations outside the BH are not influenced significantly by the presence of matter inside the BH. The coupling of the hydrodynamic evolution to the spacetime evolution with the CCZ4 method does not seem to compromise the stability of the BH evolution in any way. It is, however, necessary either to limit the fluid state at the center of the BH as described in Sec. [II] or to gradually remove the matter from the center as described above.

As a measure of accuracy, we monitor the BH mass extracted using the isolated horizon formalism. For the collapse of a spherical star, the BH has to be stationary after all matter has crossed the horizon, and the BH mass has to be exactly the ADM mass of the initial unstable star. We therefore compute the maximum deviation of the numerically extracted value from the exact one during the time interval 200–800 $M$ after apparent horizon detection. The results are reported in Table II. For the noncovariant CCZ4 simulations of the collapse, the accuracy is around 0.64–2.2% for damping parameters $0.02 \leq \kappa_1 \leq 0.1$. As we will show in Sec. [III], the error can be reduced below 0.3% by a modification of the damping terms, which allows the use of the covariant version ($\kappa_3 = 1$). Nevertheless, the standard BSSNOK and Z4c formulations are more accurate in terms of BH mass for this test.

\section*{C. Binary neutron stars with constraint-violating initial data}

We next present tests of the CCZ4 formulation when applied to merging binary NSs with constraint-violating initial data. These are probably the most demanding tests with respect to constraint violations because the initial data already contain large violations of the constraint equations.

We start by considering binaries on eccentric orbits and set up such initial data by starting with a constraint-satisfying solution representing an irrotational binary on a quasicircular orbit and then simply scale the velocity by a factor of 0.85 to make the orbit eccentric (which also speeds up the insipral). This naturally introduces a large constraint violation, thus allowing us to compare the evolution schemes under extreme but well-defined conditions. More specifically, the original initial data represent an irrotational binary system on a quasicircular orbit, with equal baryon masses of $M_b = 1.779 M_\odot$, and an initial separation of $d = 45$ km. The stars obey a polytropic EOS with $\Gamma = 2$ and $K = 123.629$, while during the evolution we use an ideal gas EOS with $\Gamma = 2$. This model is publicly available from the LORENE code.

We evolve the eccentric system with the CCZ4 formulation, using various combinations of the parameters, as well as with the BSSNOK formulation. The rest of the setup stays exactly the same, in particular the gauge conditions. Figure [IV] shows
the evolution of the Hamiltonian constraint. As one can see, the constraint violations, which are the same initially, are reduced by up to 1 order of magnitude during the inspiral when using the CCZ4 formulation. The BSSNOK formulation, on the other hand, shows a moderate growth during the inspiral. Of course, the impact of the initial constraint violation on the actual dynamics of the binary is difficult to assess. Any constraint violation is obviously a deviation from the solution of the Einstein equations, although the quantitative relation between the constraint violations and the error on the physical quantities is largely unknown. It is, however, reasonable to assume that a reduction of constraint violations will also lead to more accurate results for the physical quantities. In this respect, the CCZ4 formulation is clearly better for the case considered here. Note that the accuracy that can be achieved in this way is still limited by the constraint-satisfying component of the evolution error, so that a further reduction will not increase significantly the overall accuracy.

In order to assess how the constraint violation influences the orbital motion, we have compared the trajectories of the two NSs obtained with the CCZ4 and BSSNOK formulations by tracking the “barycenters” of the two NSs. We find that significant deviations between the two trajectories develop during the evolution while simultaneously the differences in the constraint violations grow. After one orbit, the coordinate separation already differs by 18%. This is to be expected. Once the constraints are violated, the numerical solution of the evolution system belongs to an extended set of solutions of the Einstein equations. Even starting with the same amount of constraint violation, the evolution equations for the CCZ4 and BSSNOK formulations are expected to lead to slightly different results, in the vicinity of the true Einstein solution. The only question is below which magnitude of the constraint violation the errors become tolerable. Clearly, the constraint violation introduced by the crude rescaling of the velocity is already too large to obtain meaningful results.

When comparing simulations with CCZ4 using different parameters, we find that increasing the damping parameter \( \kappa_1 \) leads to a decrease in the violations of the Hamiltonian constraint during the inspiral phase. This is indeed what one would naively expect, given that a larger \( \kappa_1 \) amounts to a smaller timescale for the damping of the constraint violations. However, for \( \kappa_1 \gtrsim 0.07 \), we find an exponential growth after the BH has formed. Hence, the optimal choice for a stable evolution seems to be \( \kappa_1 = 0.05 \). Note that this value should scale with the inverse mass of the BH; see Sec. II A. So far, we have used a damping parameter \( \kappa_2 = 0 \). We did not find any significant improvement by trying different values. On the contrary, for \( \kappa_2 = -0.5 \) the constraint damping becomes less efficient.

\[ \int_V \left( f_V \, D x^i \right) \left( f_V \, D x^i \right)^{-1} \]

where the integration volume \( V \) is suitably chosen to fully contain the selected NS, but exclude the other.
Next, we consider mergers of rotating NSs. Because self-consistent initial data for rotating NS binaries are not available (although an approach to computing such models has been proposed recently in Ref. [23]), we will show in the following that it is possible to use a short evolution with the CCZ4 scheme to convert constraint-violating initial data into self-consistent initial data. This allows us to study the influence of the additional NS spins on the spin of the final BH and the surrounding disk. Although some of these results have already been presented in Ref. [29], for completeness, we review here the behavior of the two formulations in this illustrative test.

The models we investigate are constructed in a similar way as for the eccentric case, namely, by starting from irrotational quasicircular initial data. The spin is added by simply rescaling the velocity field in the co-orbiting frame by a factor $1-s$, where $s=0$ corresponds to the original irrotational model, and $s=1$ roughly to the corotating one (see Ref. [29] for details). Naturally, this introduces constraint violations, which are, however, not as strong as for the eccentric binary. It also causes ordinary oscillations of the star, which affect only the realism of the initial conditions and are not important within the scope of this test.

The spatial distribution of the constraint violation shown in Ref. [29] is similar to that shown in Fig. 7 only the initial constraint violation is more pronounced. Figure 5 shows the evolution of the Hamiltonian constraint for various amounts of spin, with the symbols marking the time of formation of the apparent horizon. The increase of the initial constraint violation with the spin is clearly visible. However, even for the fastest-spinning model, the evolution with the CCZ4 formulation rapidly reduces the Hamiltonian constraint to a much smaller magnitude, which already after $\sim 1$ ms becomes comparable with the one obtained with the BSSNOK formulation when evolving constraint-satisfying initial data. As we will show in Sec. III D, the amount of constraint violations for the latter are tolerable. We thus conclude that at these separations an evolution time of $\sim 1$ ms with the CCZ4 formulation is sufficient to produce initial data that can be considered self-consistent. Of course, although self-consistent, the initial data may well represent a physical system which is rather different from the intended one.

D. Binary neutron stars with constraint-satisfying initial data

We now turn to investigate the behavior of merging binary NSs in quasicircular orbits. For this, we evolve the original binary star model described in the previous subsection, without reducing the linear momenta. Again, we find that the CCZ4 formulation suppresses the Hamiltonian constraint by roughly 1 order of magnitude when compared to the BSSNOK formulation, as shown in Fig. 6. Varying the damping constant $\kappa_1$ in the stable range impacts the results only marginally. Figure 6 also shows a clear periodic increase/decrease of the Hamiltonian constraint violation when using the CCZ4 formulation. We believe that this behavior is related to the movement of the refined boxes. Whenever a refined box moves, the new points have to be computed by interpolation from the coarser grid, which introduces an additional error. Indeed, the period of the variations in the constraint violations corresponds to half an orbit, which is compatible with the $\pi$ symmetry of the binary. However, to further validate this hypothesis, we perform a simulation where only the finest level consists of moving boxes, in contrast to the standard setup where the two finest levels are moving boxes. As one can see in Fig. 6 by comparing the solid black and green lines, this has some influence during inspiral. Moreover, it is most prominent at the stage where the change of the overlap of the moving boxes on the second-finest level is also large. The fact that we do not observe the periodic pattern for the BSSNOK results seems to indicate that the error due to regridding is not dominant in this case.

Since binary NS mergers are an important application of our code, we perform a computationally expensive convergence test with three resolutions, each increased by a factor of 1.5. We measure the convergence order by the same method used for the single star, only that we use the finest nonmoving refinement level instead of the finest one. Furthermore, we exclude the interior of the apparent horizon (more precisely, we exclude a coordinate sphere with the mean coordinate radius of the horizon). For the lapse function, we measure an overall convergence order of $n=1.9$, while for the rest mass density this is $n=1.6$, all measured using the $L_2$ norm. The metric determinant $\gamma$ develops a strong peak at the center of the grid shortly before the apparent horizon forms. This is normal, but complicates measuring the convergence after BH formation. Indeed, during the inspiral, we obtain a convergence order $n=1.7$ for $\gamma$, which is recovered again after the BH formation. We note that the time-dependent estimate for the convergence order of all variables fluctuates strongly during the merger (up to $n=8$), which is probably caused by the accumulated phase error. As a consequence, we cannot prove convergence for this stage. We can, however, establish con-
FIG. 7: Comparison of the local Hamiltonian constraint violations when evolving the quasicircular coalescence with the BSSNOK and CCZ4 systems. The panels depict the Hamiltonian constraint in the \((x, y)\) plane at different times: (a) \(t = 0\), initial data, (b) \(t = 6\) ms, inspiral, (c) \(t = 12\) ms, final state. The left half of each panel shows the CCZ4 results, and the right half shows the BSSNOK results. The locations of the NS barycenters are marked by the red crosses.

As reported in Table III, we find a convergence order around 1.2 for the BH properties. This is not surprising since the convergence order of the hydrodynamic evolution scheme probably reduces to 1 during the merger due to the formation of strong shocks. Nevertheless, the errors of BH mass and spin are quite small. Using Richardson extrapolation, we obtain an extrapolated total error for the values obtained at the lowest resolution, which is 0.9% for the BH mass and 0.3% for the spin. The appearance of an apparent horizon is the result of an independent search algorithm on a complex combination of the evolved quantities and, as such, not necessarily sharing the same convergence order of the evolved equations. That said, we find that the time of first appearance of an apparent horizon has a convergence order \(n = 2.1\), but is also the quantity with the largest error. The error with respect to the Richardson extrapolated time is 9% for the lowest resolution and 2% for the highest. The error introduced by the different frequency at which the apparent horizon is searched at different resolutions is much smaller and only \(\sim 0.1\)%.

In contrast to the eccentric case, the dynamics of the quasicircular system agrees well between the CCZ4 and BSSNOK formulations. To quantify this statement, we compare the mass, spin, and formation time of the BH in Table III. The agreement is better than 1%. The differences in the BH properties are thus comparable to the numerical errors of the CCZ4 simulation as determined by the convergence test. Curiously, the difference in horizon formation time is an order of magnitude smaller than the numerical errors for this particular case, although we do not expect that this holds in general. Since the constraint violations still differ by a factor \(\approx 10\) between CCZ4 and BSSNOK, one can conclude that the magnitude of constraint violations observed in the quasicircular BSSNOK evolution is tolerable, while the amount present in the eccentric case already leads to severe errors. This is a very useful notion since, as we discussed before, the relation between the constraint violation and error of physical quantities is largely unknown. We stress that the \(L_2\) norm we use to quantify the constraint violations depends on the computational volume and the fall off behavior of the constraint violations. For different setups, one has to rescale accordingly in order to make sensible comparisons.

Besides the amount of constraint violation, we are also interested in its spatial distribution. Figure 4 shows the Hamiltonian on a cut in the \((x, y)\) plane. Clearly, most of the violations are produced along the orbit of the stars. Also, the mesh refinement boundaries are clearly visible. In practice, the stars leave behind a trail of constraint violations, which is more pronounced and decays more slowly for the BSSNOK formulation. Furthermore, constraint violations travel through the computational domain and are partially reflected at each refinement boundary, for both the CCZ4 and the BSSNOK formulations. After the formation of the BH, when the system approaches a final state, the constraints exhibit a relatively stationary spiral pattern of slowly decreasing magnitude.

| Form | \(M_{BH}/M_\odot\) | \(a_{BH}\) | \(\Delta_{Form}\) | \(\Delta_{Res}\) | \(n\) |
|------|--------------------|----------|-----------------|----------------|-----|
| BSSNOK | 3.222 | 0.837 | 0.6 % | 0.5 % | 1.2 |
| CCZ4 | 3.204 | 0.840 | 0.4 % | 0.2 % | 1.2 |

TABLE III: Comparison of physical quantities at the end of the quasicircular coalescence, obtained with the BSSNOK and CCZ4 formulations. Above, \(M_{BH}\) is the mass of the final BH, \(a_{BH} = J_{BH}/M_{BH}^2\) its dimensionless spin parameter, and \(t_{BH}\) is the time when the apparent horizon is detected. The difference between the highest and lowest resolution of the CCZ4 convergence test is given by \(\Delta_{Res}\), while \(p\) is the measured convergence order. The difference between results obtained with the BSSNOK and CCZ4 formulations at the lowest resolution is denoted by \(\Delta_{Form}\).
Fig. 8: Accuracy of the gravitational wave signal in terms of the $\ell = m = 2$ multipole component of the Weyl scalar $\Psi_4$, extracted at $r \approx 664$ km. Top left: Amplitude of $\Psi_4$. Bottom left: Complex phase $\Phi$ (see main text). Top right: Residuals of the amplitude between CCZ4 simulations with different resolutions, and between BSSNOK and CCZ4 at lowest resolution. The residual between high and medium resolution is rescaled assuming a convergence order of 1.7. Bottom right: Residuals of the phase, also rescaled.

Finally, we should also remark that the relative difference in the constraint violations that we measure in the simulations reported here refers to our implementation of the CCZ4 and BSSNOK formulations and should not be considered as universal. Because a number of slightly different versions of the BSSNOK system are used by different groups, it is possible that the differences between the two formulations could also be smaller or larger when performed by other groups.

1. Gravitational wave signal

One of the most important results of binary NS merger simulations is obviously the emission of gravitational wave (GW) signals. Since prior to extraction, GWs travel into the weak-field region, crossing several refinement boundaries and becoming a small perturbation due to the $1/r$ falloff, they might be affected more strongly by numerical errors than the bulk dynamics of the merger. In particular, constraint violations could affect the GWs differently. In the following subsection, we measure the numerical accuracy of the GW signal using the CCZ4 convergence test and estimate the influence of constraint violations by comparing between the CCZ4 and the BSSNOK formulations.

For this, we extract the $\ell = m = 2$ component of the Weyl scalar $\Psi_4$ at a fixed radius $r = 664$ km. We then decompose the complex quantity $\Psi_4$ into amplitude and phase, i.e., $\Psi_4 = A \exp(i\phi)$, where $\phi$ is a continuous function of time. To compare different simulations, we measure time with respect to the time $t_{\text{AH}}$ at which the apparent horizon forms, and introduce the phase difference $\Phi(t) = \phi(t) - \phi(t_{\text{AH}})$. The amplitude and the phase are shown in the left panels of Fig. 8 for the BSSNOK and CCZ4 results. For the CCZ4 simulations, we plot the three resolutions of the convergence test, where the lowest one is identical to the one used for the BSSNOK simulation. One can clearly distinguish the inspiral phase, a first peak corresponding to the merger, and a second peak corresponding to the ringdown of the BH. The usual junk radiation inherent to the initial data can also be seen at the beginning of the evolution. In the right panels of Fig. 8 we show the residuals of amplitude and phase between different resolutions and between the CCZ4 and BSSNOK runs when performed at the lowest resolution. For the CCZ4 runs, we find errors compatible with a convergence order around 1.7 during the inspiral. During the merger, on the other hand, the convergence decreases and is lost during the ringdown phase. From the time derivative of $\Phi$, we compute the instantaneous frequency, which increases from around $\Phi \approx 7 \text{ rad ms}^{-1}$ at the end of the inspiral to $\Phi \approx 35 \text{ rad ms}^{-1}$ at the maximum of the ringdown signal. Unfortunately, the wavelength corresponding to the latter is resolved by only six coarsest grid points of the lowest resolution, and thus the signal from the ringdown is severely under-resolved. In order to demonstrate convergence of the high-frequency part of the signal, we would have to repeat the runs with much higher resolution in the weak-field region.
In the analysis of GW data using matched filtering techniques, the most important error is the phase shift during the inspiral. For our test case, we find that the total phase error until the merger is less than 0.4 rad for the lowest resolution, and 0.1 rad for the highest one. At first sight, this seems to contradict the larger relative error we obtain for the time until BH formation (compare Table III). However, by analyzing the coordinate separation of the stars barycenter, we find that the relative error of separation is larger than the error of the GW phase; i.e., the orbital period is more accurate than the decrease in separation per orbit. This is reflected in the relatively large amplitude error (see Fig. 8), since the GWs at the same phase (or time) are produced at different orbital separations.

Figure 8 also shows that the differences in the waveforms obtained with the CCZ4 and the BSSNOK formulations are generally comparable to the numerical errors, even during merger and ringdown. Since the constraint violations differ by 1 order of magnitude, we can conclude that their impact on the GW signal is also comparable to that due to numerical errors, or even smaller (the differences could as well be purely due to numerical errors other than the constraint violation). This result is rather reassuring since, to the best of our knowledge, the impact of the constraint violations on the accuracy of the GW signal has not been measured before.

Note that although the gauge condition is the same for both simulations, the coordinate separation is a gauge-dependent quantity.

FIG. 9: Comparison between the noncovariant and fully covariant CCZ4 and the noncovariant Z4c systems in evolutions of a nonrotating stable neutron star. Shown is the time evolution of the $L_2$ norm of the Hamiltonian constraint violation (top panel) and the momentum constraint violation (bottom panel).

FIG. 10: Comparison between the noncovariant and covariant versions of the CCZ4 and the noncovariant Z4c systems in evolutions of a nonrotating BH. Shown is the time evolution of the $L_2$ norm of the Hamiltonian constraint violation (top panel) and of the $\Theta$ variable (bottom panel), computed excluding the interior of the BH.

E. Comparison with the Z4c formulation

As anticipated in the Introduction, we now present a comparison of the results obtained with another conformal formulation of the Z4 system, namely the Z4c formulation proposed in Ref. [11]. To reduce the computational costs, the comparison will be carried out with the evolutions of a stable nonrotating star, of a single nonrotating BH and of an unstable NS which collapses to a BH. However, we expect that the qualitative behavior of the two formulations will extend also to binary systems either of BHs or of NSs. As far as the Z4c system is concerned, we have implemented the formulation described in Ref. [11] within the McLachlan code [20]. This requires only minor modifications in the source terms of the CCZ4 system (see Sec. II A for details about the differences between the two systems). As mentioned in Sec. II C, we use the radiative boundary conditions provided by the McLachlan code.

We note that both the CCZ4 and the Z4c formulations implement the same constraint-damping scheme [12], and we use the values of the constraint-damping parameters advocated as best suited for the Z4c formulation in Ref. [11], namely $\kappa_1 = 0.02$ and $\kappa_2 = 0.0$. Also, for both systems we monitor the same quantities, namely the behavior of the Hamiltonian and momentum constraint violations, but also of the $\Theta$ function, whose time variation measures the size of the Hamiltonian constraint violation and thus assesses the deviation of the numerical solution from the true Einstein solution. Indeed, we find this diagnostic quantity to be a very important indicator of the quality of the solution, which can be compared directly for the two conformal formulations (we recall that the $\Theta$ function is not defined for the BSSNOK formulation).

The first test involves a nonrotating stable NS, as described in Sec. II A. Overall, in the presence of matter the two systems provide an almost identical behavior and show a 2-order-
of-magnitude decrease in the constraint violations as the evolution is started. These are reported in Fig. 9, which shows both the violations in the Hamiltonian and the momentum constraints (top and bottom panels, respectively). Note that the Z4c evolution has a slightly larger violation of the Hamiltonian constraint (top panel) and a smaller one in the momentum constraints (bottom panel). Overall we find the two violations comparable.

The second test involves the evolution in vacuum of a nonrotating BH. The results are again very similar for the two systems, as one can see in Fig. 10 which reports the violation in the Hamiltonian constraint and the evolution of the Θ function (top and bottom panels, respectively). Note that while the Hamiltonian constraint is slightly smaller for the Z4c formulation, the momentum constraint is smaller for CCZ4. Both systems show small deviations in the final BH mass; see Table II.

The third comparative test consists in the collapse of an unstable TOV star, as described in Sec. III B. Figure 11 shows again the violation in the Hamiltonian constraint and the evolution of the Θ function (top and bottom panels, respectively). The only significant difference in this case is a spike in the Θ function (top and bottom panels, respectively). Note that while the Hamiltonian constraint is slightly smaller for the Z4c formulation, the momentum constraint is smaller for CCZ4. Both systems show small deviations in the final BH mass; see Table II.

Based on the results presented above, we conclude that the CCZ4 and the Z4c formulations yield very similar results in terms of their ability to damp the violations in the constraint equations. However, one important difference remains between the two systems that is, only the CCZ4 formulation with κ3 = 1 represents a version of the original Z4 system that is not only conformal but also covariant. As a result, only for this covariant formulation should one reasonably expect that the qualitative behavior of the constraint violations will remain unchanged when evolving the same system in different coordinates. Finally, given the similar behavior of the CCZ4 and of the Z4c formulations for the tests considered here, we expect that, when used in the evolution of binary NSs, the Z4c system would also yield violations that are of about 1 order of magnitude smaller than those with the BSSNOK formulation.

F. Fully covariant CCZ4 in black hole spacetimes

As a concluding section, we now discuss how it is possible to employ a covariant CCZ4 formulation, i.e., with κ3 = 1, also for spacetimes containing BH singularities. We recall that in cases where no singularity is present, as for example in the evolution of a TOV, the fully covariant CCZ4 system is stable and the standard constraint-damping prescription leads to results similar to the noncovariant CCZ4 formulation as well as to the Z4c systems (cf. Fig. 5). However, in those cases in which a BH is present, either initially or when it is formed during the evolution, the fully covariant CCZ4 system coupled with the constraint-damping scheme has shown exponentially growing modes (cf. Fig. 4 in paper I).

Even though we could not identify the exact cause of the instability (see discussion in Sec. II A), it is clear that in Eqs. (4) and (5) the constant damping coefficient κ1 is always multiplied by the lapse function α. Because our singularity-avoiding slicing reduces considerably the value of the lapse near the singularity, it is clear that the benefits introduced by the damping term κ1 are severely suppressed right there where the violations are the largest. Fortunately, these considerations suggest two new prescriptions for the damping terms. In detail, we replace the constant κ1 in Eqs. (4)–(6) with one of the following functions:

\[
\kappa_1 \rightarrow \frac{\kappa_1}{\alpha}, \quad (27)
\]

\[
\kappa_1 \rightarrow \frac{\kappa_1}{2} \left( \alpha + \frac{1}{\alpha} \right). \quad (28)
\]

In this way, the product ακ1 is not approaching zero anymore near the singularity. Note that the Z4 damping terms, i.e., the terms containing κ1, are not fully covariant anymore, but only spatially covariant, since we introduced an explicit dependency on the slicing. The main Z4 evolution equations on the other hand remain unchanged and fully covariant.

Although the two prescriptions Eqs. (27) and (28) are slightly different in their local and asymptotic behavior, they yield very similar results, and we focus on the form (27) in the following. To validate the effectiveness of the new prescription, we recompute the tests performed in the previous section and compare them with those obtained with the noncovariant version of the CCZ4 formulation (i.e., with κ3 = 0.5) and with the Z4c formulations. Since we use the same computational infrastructure, numerical methods and gauge conditions, the only differences between the two systems are the Z4 source terms, which were truncated in the noncovariant CCZ4 version and are completely removed in the Z4c system (see Eqs. (1)–(3)).

The comparison is shown in Fig. 10 which presents results obtained with two values of the damping parameter, namely κ1 = 0.1 and κ1 = 0.02, in evolutions of a single nonrotating BH. The latter allows a direct comparison with the noncovariant CCZ4 and Z4c results, and indeed the constraint violations are very similar in this case. Larger damping values lead to lower values of Θ and of the violations of the momentum constraints. Even though the two damping parameters are significantly different, the violations of the constraints change by less than 1 order of magnitude over the timescale of this evolution, i.e., 5 ms. A significant effect, however, is observed in the black hole mass, which shows deviations of 0.1% in the first case and 2.8% in the second case (see Table II).

Overall, the behavior of the covariant CCZ4 constraints matches well the noncovariant version of the CCZ4 system for the same value of the damping parameter, for example κ1 = 0.1 in Fig. 11. However, the two versions of the CCZ4 formulations differ in the value of the final BH mass after collapse, namely, the covariant one shows a difference of 1.01% with respect to the initial gravitational mass of the NS, while
the noncovariant one shows a 0.51% error. A study of the influence of different damping parameters on the values of the BH mass is presented in Table I. In practice, larger values of the damping lead to more reliable estimates of the mass; for example, $\kappa_1 = 0.17$ reduces the error to 0.23%.

We believe that the new prescriptions for the damping term Eqs. (27) and (28) are important for two distinct reasons. First, they allow for the use of a covariant CCZ4 formulation also in singular BH spacetimes. This was a limitation of our approach in paper I that has been successfully overcome. Second, these results shed some light on the behavior of the “nonprincipal part” constraint-damping terms in the CCZ4 system, although a complete and closer comparison with the Z4c results presented in Ref. [11] cannot be performed because of the different boundary conditions employed.

IV. CONCLUSIONS

We have compared numerically the performance of several conformal and traceless formulations of the Z4 system with the BSSNOK formulation in simulations of spacetimes with and without matter, in terms of the suppression of constraint violations and their impact on the accuracy of physical quantities. We successfully coupled the CCZ4 system presented in paper I to matter sources, and also found that the fully covariant CCZ4 version leads to stable evolutions for the case of NSs, while it develops instabilities as soon as a BH is present. We created a modified CCZ4 version that completely eliminates those instabilities for BH spacetimes also, and which is still covariant. In addition, we implemented the Z4c formulation described in Ref. [11] in our numerical framework and compared its properties to those of the CCZ4 formulation.

We have found that the noncovariant CCZ4 formulation introduced in paper I is stable when coupled to matter sources in simulations of stable and unstable spherical NSs, as well as of merging binary NSs. In comparison to the BSSNOK system, the CCZ4 formulation reduces the constraint violations by 1 order of magnitude for simulations of binary NSs and by 2 orders for single NSs. We have also demonstrated the convergence of our implementation for simulations of stable NSs, as well as those of binary NS mergers, with a convergence order in the range 1.2-2, mainly limited by the hydrodynamic evolution scheme. By comparing the CCZ4 and the BSSNOK evolutions, and by using the large differences in the constraint violations, we could estimate the influence of the latter on physical quantities. In particular, we could demonstrate that the impact of the constraint violations on the GW signal from the binary NS mergers is smaller than or comparable to the numerical errors.

Furthermore, a comparison of the different conformal Z4 versions, namely the noncovariant and covariant CCZ4 formulations, and the noncovariant Z4c, has shown that they have an almost identical behavior in terms of constraint violations as long as no singularity is present (e.g., stable TOV). In evolutions of BH spacetimes, or when a BH is produced as a result of a collapse, we find that values of the constraint-damping parameter larger than the ones proposed for the Z4c formulation (i.e., $\kappa_1 = 0.1$ in place of $\kappa_1 = 0.02$) lead to lower constraint violations and do not produce late-time instabilities. Finally, we have also found that the modification of the damping terms mentioned above is useful not only for a stable evolution of the covariant CCZ4 system, but also for reducing the drift in the BH mass for both CCZ4 versions.

Overall, we recommend CCZ4 as the standard formulation of the Einstein equations to be used in numerical relativity evolutions. In cases where constraint violations are problematic, e.g., when using constraint-violating initial data, the CCZ4 formulation is clearly superior. On the other hand, when using constraint-satisfying initial data, the reduction of constraint violations is accompanied by errors that are very similar to those obtained with the BSSNOK formulation. No additional computational costs are needed, and simple Sommerfeld radiative boundary conditions are sufficient to obtain stable evolutions. On the basis of the tests where we performed a direct comparison, the performance of Z4c and CCZ4 seems to be comparable. However, CCZ4 has the advantage of being covariant, while Z4c has been successfully tested with constraint-preserving boundary conditions; see Ref. [11]. In simulations of binary neutron star mergers, a main limitation of the accuracy is given by the hydrodynamic part. For this application, using higher-order schemes for the hydrodynamic equations, such as those presented in Ref. [19], might have a larger impact than the choice between CCZ4 and Z4c.

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