

Covariant and gauge-invariant metric-based gravitational-waves extraction in numerical relativity

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We revisit the problem of gravitational-wave extraction in numerical relativity with gauge-invariant metric perturbation theory of spherical spacetimes. Our extraction algorithm allows the computation of even-parity (Zerilli-Moncrief) and odd-parity (Regge-Wheeler) multipoles of the strain from a $(3+1)$ metric without the assumption that the spherical background is in Schwarzschild coordinates. The algorithm is validated with a comprehensive suite of three-dimensional problems including fluid (f -modes) and spacetime (w -modes) perturbations of neutron stars, gravitational collapse of rotating neutron stars, circular binary black holes mergers and black hole dynamical captures, and binary neutron star mergers. We find that metric extraction is robust in all the considered scenarios and delivers waveforms of overall quality similar to curvature (Weyl) extraction. Metric extraction is particularly valuable in identifying waveform systematics for problems in which the reconstruction of the strain from the Weyl multipoles is ambiguous. Direct comparison of different choices for the gauge-invariant master functions show very good agreement in the even-parity sector. Instead, in the odd-parity sector, assuming the background in Schwarzschild coordinates can minimize gauge effects related to the use of the Γ -driver shift. Moreover, for optimal choices of the extraction radius, a simple extrapolation to null infinity can deliver waveforms compatible to Cauchy-characteristic extrapolated waveforms.

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I. INTRODUCTION

Numerical relativity is the main approach for the computation of gravitational waves (GWs) from dynamical spacetimes with black holes and neutron stars. Most of the successful simulation methods rely on the $(3+1)$ formulation of general relativity, which turns Einstein equations into a Cauchy problem (with constraints) for the description of globally hyperbolic spacetimes, e.g., Ref. [1]. The computation of GWs from these numerically generated spacetimes is not straightforward as it requires specific

algorithms to identify the gauge-invariant multipoles of the radiation from the metric fields. These procedures introduce part of the systematic uncertainties that affect numerical waveforms.

Waveform extraction in $(3+1)$ numerical relativity¹ can be implemented using the metric-based perturbation theory of spherically symmetric spacetimes proposed by Regge and Wheeler [2], Zerilli [3], and Moncrief [4,5]. The original formalism adopts a background metric in Schwarzschild coordinates and the Regge-Wheeler (RW) gauge for the perturbations. Gauge-invariant perturbations were introduced in Refs. [4,5]. A covariant formalism (spherical background in generic coordinates) perturbations was later proposed by Gerlach and Sengupta [6] and further developed by other authors [7–10].

Gauge-invariant metric-based GW extraction algorithms have been extensively used in numerical relativity;

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¹We strictly refer to simulations with Cauchy foliations.

see, e.g., Refs. [11–18]. Most of these algorithms assume Schwarzschild coordinates for the background metric [11,12], although the latter do not necessarily match the coordinates of the numerically generated spacetimes at finite extraction radii. However, waveform extraction algorithms can be formulated in *any* coordinate system for the background metric by identifying the areal radius r of the 2-spheres in the numerically generated spacetime [9,10]. Pazos *et al.* [13] consider a metric-based extraction algorithm based on gauge-invariant and coordinate-independent *odd-parity* perturbations (axial sector). Their $(3+1)$ -dimensional $[(3+1)\text{D}]$ simulations of a perturbed Kerr-Schild black hole demonstrate that the coordinate-independent approach has significant advantages over the use of Schwarzschild background. Baiotti *et al.* [15] consider a similar algorithm based on gauge-invariant and coordinate-independent *even-parity* perturbations (polar sector) and a preliminary application in $(3+1)\text{D}$ simulations of a perturbed nonrotating neutron star. Buonanno *et al.* [16] (see their Appendix) present a binary black hole merger waveform computed with a gauge-invariant and coordinate-independent metric-based algorithm, but no details are given on the implementation. To our knowledge, algorithms based on the gauge-invariant and coordinate-independent formalism and including both even and odd perturbations have not been assessed for other problems.

Following the binary black hole breakthrough [19–21], other GW extraction methods have gained more popularity than metric-based algorithms. Algorithms using the Newmann-Penrose (NP) (curvature-based) formalism [22] are routinely used to extract GWs at finite coordinate radii in the “wave zone” of the simulated spacetime, e.g., Refs. [18,23–27]. Direct comparisons of waveforms extracted with metric- and curvature-based algorithms are discussed in, e.g., Refs. [14–16,18,28,29] for various problems including isolated neutron stars, gravitational collapse, and black hole mergers. These works find that the two approaches broadly agree, although curvature-based algorithms appear more robust than metric-based algorithms. The latter are more susceptible to numerical noise and gauge effects leading to waveforms with larger spurious high-frequency oscillations. Curvature-based algorithms also have drawbacks. They compute the multipoles of Weyl’s ψ_4 pseudoscalar, which are asymptotically connected to the strain multipoles by $\ddot{h}(t) = \psi_4(t)$. The time integration of the latter equation is known to be problematic: various sources of numerical error in the simulations contribute to large secular nonlinear drifts in the integrated strain data (random walk effects for time-domain integrations and spectral leakage in the frequency domain.) The frequency-domain integration with high-pass filters proposed in Ref. [30] can significantly reduce spurious effects in the oscillatory modes, but it requires the identification of a cutoff frequency. Such a frequency is easily found in terms of the initial data orbital frequency for

simulations of circular binary mergers, but its determination for noncircular mergers and binary scattering waveforms is ambiguous [31]. As a result, the uncertainty introduced by the choice of the cutoff frequency significantly affects the waveform morphology in quantitative modeling studies [31]. Similarly, nonoscillatory modes like those dominating waveforms from gravitational collapse can be challenging to integrate [18,32].

A common issue of the above metric- and curvature-based approaches is that the numerical waveforms are not rigorously computed at future null infinity ($\mathcal{I}^+$). Waveforms extracted at 2-spheres of finite coordinated radius should be extrapolated to $\mathcal{I}^{+2}$ using an approximate retarded time, e.g., Refs. [26,33–35]. Alternatively, GW extraction at $\mathcal{I}^+$ can be performed with the Cauchy-characteristic extraction (CCE) algorithm [36–41]. In this approach, $(3+1)\text{D}$ data from a world tube in the interior of the simulated Cauchy domain is propagated to null infinity using a characteristic evolution (null-cones formulation) of Einstein equations. Note that also CCE data retain a dependence on the extraction radius of the world tube data and are affected by systematics introduced by the timelike boundary of the Cauchy evolution, e.g., Ref. [42].

More consistent approaches to the computation of GWs require to directly incorporate $\mathcal{I}^+$ in the computational domain, thus adding significant mathematical and numerical complexity to the problem. Numerical-relativity simulations with the Cauchy-characteristic matching [36,43–46] achieve this goal by joining an inner world tube with a characteristic evolution that provides both waveforms and boundary conditions at $\mathcal{I}^+$; see Ref. [47] for a review. While significant progress has been made with Cauchy-characteristic matching, simulations of astrophysical scenarios are still limited. Yet another option is to consider evolution schemes for Einstein equations with hyperboloidal foliations [48–53]. Recent efforts in this direction appear promising [54–57], but obtaining a robust hyperboloidal framework for $(3+1)$ numerical relativity remains an open problem.

In this paper, we revisit the problem of gravitational-wave extraction with the gauge-invariant and coordinate-independent metric-based formalism. The motivation behind our work is threefold. First, metric-based algorithms can be a valuable option to study systematics effects in numerical waveforms especially for problems in which ψ_4 integration is a main source of uncertainty and more sophisticated methods may not be yet available or sufficiently robust. Second, the performances of coordinate-independent metric-based extraction in various computational problems relevant in astrophysical simulations have not yet been studied in detail. Third, the GW multipole data extracted here offer a way to investigate

²In general, the extrapolation procedure allows one to estimate an uncertainty of the finite-radius extraction.

GW extraction at $\mathcal{I}^+$ based on hyperboloidal foliations. A companion paper [58] describes a first effort that employs a perturbative hyperboloidal evolution of world tube data to extrapolate GW to $\mathcal{I}^+$.

The paper is organized as follows. Section II gives a comprehensive description of gauge-invariant coordinate-independent metric-based algorithms. General expressions for the odd and even-parity master functions are explicitly reported for a background in generic coordinates and including time dependence. Section III describes the wave extraction algorithm and the different choices of the areal radius. Section IV describes our implementation in the GR-Athena++ code and the setup of the $(3+1)$ D simulations. The following sections discuss numerical results for a suite of $(3+1)$ D problems: perturbations of neutron stars (Sec. V), gravitational collapse of rotating neutron stars (Sec. VI), circular and eccentric binary black holes mergers (Sec. VII), and binary neutron star mergers (Sec. VIII). The paper concludes with a summary of our findings and recommendations on the use of metric-based extraction.

The paper uses geometric units $c = G = 1$ unless explicitly specified. All conventions are summarized in Appendix A. Appendix B provides further details on the numerical implementation. Appendix C provides further results on a simple and yet effective extrapolation of metric waveforms to $\mathcal{I}^+$.

II. MULTIPOLAR DECOMPOSITION OF WAVE-ZONE METRIC AND MASTER FUNCTIONS

In the metric-based extraction formalism, the wave-zone metric is decomposed according to the gauge-invariant and coordinate-independent perturbation theory of spherical spacetimes of Regge-Wheeler-Zerilli-Moncrief and others (hereafter, RWZ). Here, we assume that the spherical background metric has been identified (see Sec. III) and discuss how to build the gauge-invariant Zerilli-Moncrief (even parity, $\Psi_{\ell m}^{(e)}$) and Regge-Wheeler (odd parity, $\Psi_{\ell m}^{(o)}$) master functions from a numerically generated $(3+1)$ -metric. The master functions are independent of the coordinates in which the background spacetime is expressed. Gravitational waves are expressed as a $s = -2$ spin-weighted spherical harmonics expansion with the even- and odd-parity master functions:

$$\begin{aligned} h_+ - ih_\times &= \frac{1}{D_L} \sum_{\ell \geq 2} \sum_{m=-\ell}^{\ell} h_{\ell m}^{(-2)} Y_{\ell m} \\ &= \frac{1}{D_L} \sum_{\ell \geq 2} \sum_{m=-\ell}^{\ell} \sqrt{\frac{(\ell+2)!}{(\ell-2)!}} \\ &\quad \times \left(\Psi_{\ell m}^{(e)} + i \Psi_{\ell m}^{(o)} \right)^{(-2)} Y_{\ell m}. \end{aligned} \quad (1)$$

The 4-metric $g_{\mu\nu}$ of a perturbed spacetime is given by the spherical background ${}^{(4)}g_{\mu\nu}^o$ plus a nonspherical perturbation, $h_{\mu\nu}$. The background metric can be time dependent, and it is fully characterized by the mass of the central object M , which is a time-independent quantity; see Appendix A. The perturbation is decomposed in spherical tensor harmonics and, due to the rotational symmetry of the background, decouples in even- and odd-parity parts:

$${}^{(4)}g_{\mu\nu} = {}^{(4)}g_{\mu\nu}^o + \sum_{\ell=2}^{\infty} \sum_{m=-\ell}^{\ell} \left(h_{\text{even}\mu\nu}^{(\ell m)} + h_{\text{odd}\mu\nu}^{(\ell m)} \right). \quad (2)$$

The even-parity perturbation is

$$h_{\text{even}\mu\nu}^{(\ell m)} = \begin{pmatrix} h_{AB} Y_{\ell m} & h_A Y_c^{(\ell m)} \\ h_A Y_c^{(\ell m)} & r^2 (K \sigma_{ab} Y_{\ell m} + G Y_{ab}^{(\ell m)}) \end{pmatrix}, \quad (3)$$

and h_{AB} , h_A , K , and G are the *even-parity multipoles* with indices $A, B = 0, 1$. The suffix (ℓm) in these fields is omitted for brevity. Each multipole is a function of the background coordinates x^A of the Lorentzian background 2-metric g_{AB} . If one chooses, for example, the areal (Schwarzschild) radius, then $x^1 = r$. We refer the reader to Appendix A for the definition of the even-parity tensor spherical harmonics $Y_{\ell m}$, $Y_a^{(\ell m)}$, $Y_{ab}^{(\ell m)}$ with indices $a, b = 2, 3$.

The notation here mainly follows Gundlach and Martin-Garcia [7] and Martel and Poisson [10]. The functions h_A that are indicated as j_A in Martel and Poisson [10], while we follow here the original notation of Regge and Wheeler [2]. Working in Schwarzschild coordinates, Regge and Wheeler [2] use for the multipoles the symbols H_0 , H_1 , H_2 . The latter are related to ours via $h_{00} \equiv N H_0$, $h_{01} \equiv H_1$, and $h_{11} \equiv H_2/N$, where N is the background function defined in Appendix A. The function K differs from the one used by Regge and Wheeler [2],

$$K_{\text{RW}} := K + \frac{\lambda}{2} G, \quad (4)$$

because of the different convention used there for the $Y_{ab}^{(\ell m)}$ basis. Note that the Regge-Wheeler gauge corresponds to the choice $h_A = 0 = G$.

The odd-parity perturbation is

$$h_{\text{odd}\mu\nu}^{(\ell m)} = \begin{pmatrix} 0 & H_A S_c^{(\ell m)} \\ H_A S_c^{(\ell m)} & H S_{ab}^{(\ell m)} \end{pmatrix}, \quad (5)$$

where H_A and H are *odd-parity multipoles*, and again (ℓm) is omitted. We refer the reader to Appendix A for the definition of the odd-parity tensor spherical harmonics $S_a^{(\ell m)}$, $S_{ab}^{(\ell m)}$.

The notation used here is close to that of Gundlach and Martin-Garcia [7] but uses uppercases to avoid clashes with the even-parity functions and additional superscripts. Comparing our notation to Martel and Poisson [10], those authors use the symbols h_A and h_2 for our H_A and H , respectively. In turn, Martel and Poisson [10] notation follows closely the notation of Regge and Wheeler [2] except that the function h_2 in the latter paper differs of a minus sign due to a sign difference in the definition of $S_a^{(\ell m)}$ [see Eq. (A13b)]. Note that the Regge-Wheeler gauge corresponds to the choice $H = 0$.

The multipoles $h_{AB}, h_A, K, G, H_A, H$ are in general gauge dependent. We detail below the construction of gauge-invariant multipoles and the RWZ master functions.

A. Gauge-invariant multipoles

For $\ell \geq 2$, it is always possible to build gauge-invariant metric multipoles starting from the multipolar decomposition given above. Using the notation originally introduced by Gerlach and Sengupta [6] (see also the work by Gundlach and Martin-Garcia [7]), the gauge-invariant *even-parity* metric perturbations are given by [(ℓm) omitted]

$$\kappa_{AB} := h_{AB} - (\nabla_A p_B + \nabla_B p_A) \quad (6)$$

$$\kappa := K_{\text{RW}} - 2 \frac{\nabla_A r}{r} p_B g^{AB}, \quad (7)$$

with the quantity

$$p_A := h_A - \frac{1}{2} r^2 \nabla_A G. \quad (8)$$

In the most general case of a *time-dependent background*, the gauge-invariant multipoles can be expressed in terms of those defined by Eq. (3),

$$\begin{aligned} \kappa = K_{\text{RW}} - \frac{1}{r} \{ & \dot{r}(2h_0 - r^2 \partial_t G) g^{00} + [\dot{r}(2h_1 - r^2 \partial_r G) \\ & + (2h_0 - r^2 \partial_t G)] g^{01} + (2h_1 - r^2 \partial_r G) g^{11} \}, \end{aligned} \quad (9a)$$

$$\begin{aligned} \kappa_{00} = h_{00} - 2\partial_t h_0 + 2(\Gamma_{00}^0 h_0 + \Gamma_{00}^1 h_1) + 2r\partial_t r \partial_t G \\ + r^2(\partial_t^2 G - \partial_t \Gamma_{00}^0 - \Gamma_{00}^1 \partial_r G), \end{aligned} \quad (9b)$$

$$\begin{aligned} \kappa_{01} = h_{01} - \partial_t h_1 - \partial_r h_0 + r\dot{r}\partial_r G + r\partial_t G \\ + 2(\Gamma_{01}^0 h_0 + \Gamma_{01}^1 h_1) + r^2(\partial_t \partial_r G - \Gamma_{01}^0 \partial_t G - \Gamma_{01}^1 \partial_r G), \end{aligned} \quad (9c)$$

$$\begin{aligned} \kappa_{11} = h_{11} - 2\partial_r h_1 + 2(\Gamma_{11}^0 h_0 + \Gamma_{11}^1 h_1) + 2r\partial_r G \\ + r^2(\partial_r^2 G - \Gamma_{11}^0 \partial_t G - \Gamma_{11}^1 \partial_r G), \end{aligned} \quad (9d)$$

where t is the global time coordinate, r is the areal radius, $\dot{r} = dr/dt$, and Γ_{BC}^C are the Christoffel's symbols of the background 2-metric g_{AB} . For completeness, we explicitly write the gauge-invariant multipoles for the case of a time-dependent background,

$$\kappa = K_{\text{RW}} - \frac{2}{r} \left[\left(h_1 - \frac{1}{2} r^2 \partial_r G \right) g^{11} + \left(h_0 - \frac{1}{2} r^2 \partial_t G \right) g^{01} \right], \quad (10)$$

and

$$\begin{aligned} \kappa_{00} = h_{00} - 2\partial_t h_0 + 2(\Gamma_{00}^0 h_0 + \Gamma_{00}^1 h_1) \\ + r^2(\partial_t^2 G - \Gamma_{00}^0 \partial_t G - \Gamma_{00}^1 \partial_r G), \end{aligned} \quad (11a)$$

$$\begin{aligned} \kappa_{01} = h_{01} - \partial_r h_0 - \partial_t h_1 + 2(\Gamma_{01}^0 h_0 + \Gamma_{01}^1 h_1) + r\partial_t G \\ + r^2(\partial_t \partial_r G - \Gamma_{01}^0 \partial_t G - \Gamma_{01}^1 \partial_r G) \end{aligned} \quad (11b)$$

$$\begin{aligned} \kappa_{11} = h_{11} - 2\partial_r h_1 + 2(\Gamma_{11}^0 h_0 + \Gamma_{11}^1 h_1) + 2r\partial_r G \\ + r^2(\partial_r^2 G - \Gamma_{11}^0 \partial_t G - \Gamma_{11}^1 \partial_r G). \end{aligned} \quad (11c)$$

The tensor κ_{AB} is called $\hat{H}_{ab}$ in Ref. [9] [see, e.g., their Eq. (16)] and $\tilde{h}_{ab}$ in the work by Martel and Poisson [10] (note also the different convention for the indices).

The gauge-invariant *odd-parity* perturbation can be constructed from the odd-parity scalar H and one-form H_A perturbations [6,8],

$$\kappa_A := H_A - \frac{1}{2} \nabla_A H + H \frac{\nabla_A r}{r}. \quad (12)$$

In terms of the multipoles of Eq. (5), the gauge-invariant odd-parity multipoles are

$$\kappa_0 = H_0 - \frac{1}{2} \partial_t H + H \frac{\dot{r}}{r}, \quad (13a)$$

$$\kappa_1 = H_1 - \frac{1}{2} \partial_r H + \frac{H}{r}. \quad (13b)$$

B. Even-parity master function

We discuss here the computation of the Zerilli-Moncrief master function from the even-parity multipoles h_{AB}, h_A, G, K . The even-parity master function implemented in most of the literature follows the computation of Moncrief [4,5]. The function is gauge invariant, but not coordinate independent, since its derivation assumes that the background metric is explicitly written in Schwarzschild coordinates. We briefly review its expression below. In the most general case, the construction of the gauge-invariant master function is explained in the work by Sarbach and Tiglio [9] and Martel and Poisson [10], which are the only papers where

such an invariant expression is reported. Here, we additionally present, for the first time, its explicit expression in terms of the multipoles $h_{AB}, h_A, K, G, H_A, H$. These multipoles are those directly computed from the 3-metric, as detailed in Sec. III.

For a background in Schwarzschild coordinates, the background 2-metric is $g_{01} = 0, g_{00} \equiv -S := -(1 - 2M/r)$ and $g_{11} = -1/g_{00}$. The mass is then [cf. Eq. (A8)]

$$M = \frac{r}{2}(1 - S). \quad (14)$$

The even-parity master function reads

$$Q_+ = \frac{1}{\Lambda} \sqrt{\frac{2(\ell-1)(\ell+2)}{\ell(\ell+1)}} \{ \ell(\ell+1) S(r^2 \partial_r G - 2h_1) + 2rS(Sh_{11} - r\partial_r K) + r\Lambda K \}, \quad (15)$$

where

$$\Lambda = (\ell-1)(\ell+2) + \frac{6M}{r}. \quad (16)$$

Only the multipoles h_{11}, h_1, G , and K are needed to compute the even-parity master Q_+ function. Note that our Q_+ is indicated as Q in Refs. [4,5].

The even-parity master function in generic coordinates and in terms of the gauge-invariant multipoles is

$$\Psi^{(e)} = \frac{r}{\lambda} \left[\kappa + \frac{2r}{(\lambda-2)r + 6M} (r^A r^B \kappa_{AB} - r r^A \partial_A \kappa) \right], \quad (17)$$

where the suffix (ℓm) is omitted and the vector r^A is defined in Appendix A. This equation can be found in the work by Martel and Poisson [10], but it is equivalent to the combination of Eqs. (20) and (25)–(27) of Sarbach and Tiglio [9]. In the latter reference, the even-parity function is simply called Ψ . The latter differs from ours by a minus sign, i.e., $\Psi = -\Psi^{(e)}$. Since $r^A = (g^{01}, g^{11})$, Eq. (17) can also be written as

$$\Psi^{(e)} = \frac{r}{\lambda} \left\{ \kappa + \frac{2r}{(\lambda-2)r + 6M} \left[(g^{11})^2 \kappa_{11} + 2g^{11} g^{01} \kappa_{01} + (g^{01})^2 \kappa_{00} - r g^{01} \partial_t \kappa - r g^{11} \partial_r \kappa \right] \right\}. \quad (18)$$

The final expression for $\Psi^{(e)}$ is obtained by replacing the gauge-invariant variables κ and κ_{AB} with the multipoles h_{AB}, h_A, G, K . For a *time-independent background* and using Eq. (10), one obtains

$$\begin{aligned} \Psi_{\text{static}}^{(e)} = \frac{r}{\lambda} \left\{ K_{\text{RW}} - \frac{2}{r} \left[\left(h_1 - \frac{1}{2} r^2 \partial_r G \right) g^{11} + \left(h_0 - \frac{1}{2} r^2 \partial_t G \right) g^{01} \right] + \frac{2r}{(\lambda-2)r + 6M} \right. \\ \left[(g^{01})^2 h_{00} + 2g^{01} g^{11} h_{01} + (g^{11})^2 h_{11} \right. \\ + \frac{1}{r} [-r(g^{01})^3 \partial_r g_{00} + 2r g^{11} (g^{00} g^{11} \partial_r g_{01} + \partial_r g^{01}) + g^{01} g^{11} (-2 + 2r g^{00} \partial_r g_{00} + r g^{11} \partial_r g_{11})] h_0 \\ + \frac{1}{r} [2(g^{11})^2 (-1 + r g^{01} \partial_r g_{01}) + r(g^{11})^3 \partial_r g_{11} + r g^{11} (g^{01})^2 \partial_r g_{00} + 2r g^{11} \partial_r g^{11}] h_1 \\ - \frac{1}{2} r g^{11} [2g^{11} (-1 + r g^{01} \partial_r g_{01}) + r(g^{11})^2 \partial_r g_{11} + r(g^{01})^2 \partial_r g_{00} + 2r \partial_r g^{11}] \partial_r G \\ + \frac{1}{2} r [r(g^{01})^3 \partial_r g_{00} - 2r g^{11} (g^{00} g^{11} \partial_r g_{01} + \partial_r g^{01}) - g^{01} g^{11} (-2 + 2r g^{00} \partial_r g_{00} + r g^{11} \partial_r g_{11})] \partial_t G \\ \left. \left. - r g^{11} \partial_r K_{\text{RW}} - r g^{01} \partial_t K_{\text{RW}} \right] \right\}. \quad (19) \end{aligned}$$

Note that one needs to compute just first order derivatives of the multipoles, i.e., $\partial_r G, \partial_t G, \partial_r K$, and $\partial_t K$, and the inverse background metric. In the most general case of a time-dependent background, the even-parity master function reads

$$\begin{aligned} \Psi^{(e)} = \Psi_{\text{static}}^{(e)} + \frac{r}{\lambda} \left\{ -\frac{2\dot{r}}{r} \left[\left(h_0 - \frac{1}{2} r^2 \partial_t G \right) g^{00} + \left(h_1 - \frac{1}{2} r^2 \partial_r G \right) g^{01} \right] \right. \\ + \frac{2r}{(\lambda-2)r + 6M} \left[\dot{r} [\dot{r}(g^{00})^2 + 2g^{00} g^{01}] h_{00} + 2\dot{r} [\dot{r} g^{00} g^{01} + (g^{01})^2 + g^{00} g^{11}] h_{01} + \dot{r} [\dot{r}(g^{01})^2 + 2g^{01} g^{11}] h_{11} \right. \\ + \frac{1}{r} [2r(g^{01})^3 \partial_t g_{01} + 2r g^{01} \partial_t g^{01} + [-r g^{00} (g^{11})^2 + 2r g^{11} (g^{01})^2] \partial_t g_{11} + r(g^{01})^2 g^{00} \partial_t g_{00}] h_0 \\ \left. \left. + g^{01} [(g^{01})^2 \partial_t g_{00} + 2g^{01} g^{11} \partial_t g_{01} + (g^{11})^2 \partial_t g_{11}] h_1 - \frac{r^2 g^{01}}{2} [2g^{01} g^{11} \partial_t g_{01} + (g^{01})^2 \partial_t g_{00} + (g^{11})^2 \partial_t g_{11}] \partial_r G \right] \right\} \end{aligned}$$

$$\begin{aligned}
& + \frac{r^2}{2} [-2(g^{01})^3 \partial_t g_{01} - 2g^{01} \partial_t g^{01} - (g^{01})^2 g^{00} \partial_t g_{00} + g^{11} (g^{11} g^{00} - 2(g^{01})^2) \partial_t g_{11}] \partial_t G \\
& + \frac{\dot{r}}{r} \left[r \dot{r} (g^{00})^3 \partial_t g_{00} + 2r g^{11} \partial_r g^{00} + 2r g^{01} (\partial_r g^{01} + \partial_t g^{00} + \dot{r} \partial_r g^{00}) + r (g^{01})^3 (2 \partial_t g_{11} + \dot{r} \partial_r g_{11}) + 2r g^{00} \partial_t g^{01} \right. \\
& + 2(g^{01})^2 (-2 + r g^{11} \partial_r g_{11}) + (g^{00})^2 [-2\dot{r}^2 + r \dot{r} g^{01} (\partial_r g_{00} + 2 \partial_t g_{01}) + 2r (g^{01} \partial_t g_{00} + g^{11} \partial_r g_{00})] - 2g^{00} g^{11} \\
& + \dot{r} g^{00} [2r \partial_t g^{00} - 6g^{01} + r (g^{01})^2 (2 \partial_r g_{01} + \partial_t g_{11})] + 4r g^{00} g^{01} (g^{01} \partial_t g_{01} + g^{11} \partial_r g_{11}) \left. \right] \left(h_0 - \frac{1}{2} r^2 \partial_t G \right) \\
& + \frac{\dot{r}}{r} \left[-2\dot{r}^2 g^{00} g^{01} + 2r (g^{01})^3 \partial_r g_{00} + 2r (g^{01})^2 (g^{00} \partial_t g_{00} + 2g^{11} \partial_r g_{01}) + 2r g^{11} (\partial_r g^{01} + g^{00} g^{11} \partial_t g_{11}) \right. \\
& + 2g^{01} [r (\partial_r g^{11} + \partial_t g^{00}) + g^{11} (-3 + 2r g^{00} \partial_t g_{01}) + r (g^{11})^2 \partial_r g_{11}] + r \dot{r} (g^{01})^3 (2 \partial_r g_{01} - \partial_t g_{11}) \\
& + r \dot{r} (g^{00})^2 [g^{01} \partial_t g_{00} - g^{11} (\partial_r g_{00} - 2 \partial_t g_{01})] + \dot{r} (g^{01})^2 (-4 + r g^{11} \partial_r g_{11}) + 2r \dot{r} g^{01} \partial_r g^{01} \\
& + 2\dot{r} g^{00} [r \partial_t g^{01} + r (g^{01})^2 \partial_r g_{00} - g^{11} + r g^{01} g^{11} \partial_t g_{11}] \left. \right] \left(h_1 - \frac{1}{2} r^2 \partial_r G \right) \\
& - r \dot{r} (g^{00} \partial_t K_{\text{RW}} + g^{01} \partial_r K_{\text{RW}}) + 2\ddot{r} (\dot{r} g^{00} + g^{01}) \left[\left(h_0 - \frac{1}{2} r^2 \partial_t G \right) g^{00} + \left(h_1 - \frac{1}{2} r^2 \partial_r G \right) g^{01} \right] \Bigg\}. \quad (20)
\end{aligned}$$

This $\Psi^{(e)}$ is the “natural” invariant function, being proportional to the multipole of the GW strain and differs from the Q_+ . The two master functions are related by a normalization factor,

$$\begin{aligned}
Q_+ &= \sqrt{2(\ell+2)(\ell+1)\ell(\ell-1)} \Psi^{(e)} \\
&= \sqrt{2\lambda(\lambda-2)} \Psi^{(e)}. \quad (21)
\end{aligned}$$

Note also that $\Psi^{(e)}$ can be computed in two ways. Either one uses expression Eq. (20), where just the first-order derivative (in time and space) of the metric multipoles G and K appears, or one uses expression Eq. (17), where the computation of the second time derivative of the metric multipoles G is required. In our implementation, we opt for the first approach, and we set the terms proportional to $\ddot{r}$ to zero (see Appendix B).

C. Odd-parity gauge-invariant multipoles

We discuss here the computation of the Regge-Wheeler master function from the odd-parity multipoles H_A , H . The first calculation is presented in Moncrief [4], and it is expressed in Schwarzschild coordinates. Other definitions were given, e.g., in the work by Cunningham *et al.* [59]; see the work by Martel and Poisson [10] and below for a comparison of definitions.

For a background expressed in Schwarzschild coordinates, the odd-parity master function of Moncrief [4] is

$$Q_\times := g^{AB} \kappa_B \frac{\nabla_A r}{r} = \frac{1}{r} \left(1 - \frac{2M}{r} \right) \left[H_1 - \frac{r^2}{2} \partial_r \left(\frac{H}{r^2} \right) \right]. \quad (22)$$

Note that this quantity is called Q in Ref. [4].

The odd-parity master function in terms of the gauge-invariant odd-parity multipoles is

$$\Psi^{(o)} = \frac{r^3}{\lambda-2} \epsilon^{BA} \nabla_A \left(\frac{\kappa_B}{r^2} \right), \quad (23)$$

where the suffix (ℓm) is omitted. By explicitly expanding the covariant derivative, one obtains

$$\Psi^{(o)} = \frac{1}{\lambda-2} \frac{1}{\sqrt{g}} [r(\partial_t \kappa_1 - \partial_r \kappa_0) + 2(\kappa_0 - \kappa_1 \dot{r})]. \quad (24)$$

Interestingly, one finds the same expression in terms of the odd-parity multipoles used in the direct decomposition of the spacetime,

$$\Psi^{(o)} = \frac{1}{\lambda-2} \frac{1}{\sqrt{g}} [r(\partial_t H_1 - \partial_r H_0) + 2(H_0 - H_1 \dot{r})]. \quad (25)$$

In Schwarzschild coordinates,³ Eq. (25) reduces to the known result [60]

$$\Psi_{\text{static}}^{(o)} = \frac{1}{\lambda-2} r \left[\partial_t H_1 - r^2 \partial_r \left(\frac{H_0}{r^2} \right) \right]. \quad (26)$$

This $\Psi^{(o)}$ is the invariant function proportional to the multipole of the GW strain. Moncrief’s $Q_\times$ is related to $\Psi_{\text{static}}^{(o)}$ by the equation

³Or any time-independent background with $g = 1$, e.g., Schwarzschild with the retarded/advanced time coordinates, $t \pm r$.

$$\partial_t \Psi^{(o)} = -Q_\times + \frac{16\pi}{\lambda - 2} \frac{r}{g_{rr}^{(4)o}} T_1^{(\ell m)}, \quad (27)$$

where $T_1^{(\ell m)}$ is the component of the odd-parity matter-source vector; see Ref. [60] for more details. In Regge-Wheeler gauge ($H \equiv 0$), the $Q_\times$ master function coincides with the original choice of Regge and Wheeler [2]. Note that $\Psi^{(o)}$ and $Q_\times$ have different dimensions and satisfy Regge-Wheeler equations that differ in the source terms. Yet another choice is the master function $\tilde{\Psi} \equiv \lambda(\lambda - 2)\Psi^{(o)}$ introduced by Cunningham *et al.* [59].

The master function $\Psi^{(o)}$ can be computed in two ways: either using expression Eq. (25), where just first order derivative of the metric multipoles H_0 and H_1 (in space and time respectively) appear, or using expression Eq. (24), where the computation of the second time derivatives of the metric multipoles κ_A is required. In our implementation, we opt for the first approach.

III. WAVE EXTRACTION ALGORITHM

We describe here the wave extraction algorithm to compute the master functions for the GW strain, Eq. (1). Assuming a numerical spacetime generated by a $(3+1)$ D numerical-relativity simulation in Cartesian coordinates $X^i = (x, y, z)$, a wave zone is first identified in the computational domain. The wave zone is populated with extraction spheres at various radii $R = \sqrt{x^2 + y^2 + z^2}$. The radial coordinate R is asymptotically interpreted as the isotropic radius of the asymptotically flat spacetime and is not the areal radius. The main steps of the algorithm are as follows:

- Interpolate the $(3+1)$ -metric to the extraction sphere and transform to coordinates (R, θ, ϕ) .
- Compute the areal radius r and perform the coordinate transformation to (r, θ, ϕ) .
- Compute the background metric g_{AB} at the extraction sphere.
- Compute the even- and odd- parity (gauge-dependent) multipoles as tensor spherical harmonics projections of the $(3+1)$ -metric at the extraction sphere.
- Compute the gauge-invariant master functions from Eqs. (15), (19), (20), (22), (25), and (26).

Details about steps a–d are given in the following. Table I summarizes notation and properties of the master functions considered in step e.

TABLE I. Summary of RWZ master functions.

Background	Even	Equation	Odd	Equation
Schwarzschild	Q_+	(15)	$Q_\times$	(22)
Static	$\Psi_{\text{static}}^{(e)}$	(19)	$\Psi_{\text{static}}^{(o)}$	(26)
General	$\Psi^{(e)}$	(20)	$\Psi^{(o)}$	(25)

A. $(3+1)$ -metric at the extraction sphere

The $(3+1)$ -metric γ_{ij} , shift vector β_i , and lapse function α in Cartesian coordinates are interpolated to the extraction sphere with coordinates (R, θ, ϕ) together with their spatial Cartesian derivatives and time derivatives. The components are then transformed to spherical polar coordinates using the usual transformation matrix

$$O = \begin{pmatrix} \sin \theta \cos \phi & R \cos \theta \cos \phi & -R \sin \theta \sin \phi \\ \sin \theta \sin \phi & R \cos \theta \sin \phi & R \sin \theta \cos \phi \\ \cos \theta & -R \sin \theta & 0 \end{pmatrix}. \quad (28)$$

This gives the components

$$\alpha, \beta_R, \beta_\theta, \beta_\phi, \gamma_{RR}, \gamma_{R\theta}, \gamma_{R\phi}, \gamma_{\theta\theta}, \gamma_{\theta\phi}, \gamma_{\phi\phi}, \quad (29)$$

at the extraction sphere. The radial derivatives with respect to R are computed from the Cartesian derivatives by defining the unit vector $n_i = X_i/R$ and, for each function $f \equiv f(x, y, z)$,

$$\begin{aligned} \partial_R f &= \delta^{ij} n_i \partial_j f = \hat{n}_x \partial_x f + \hat{n}_y \partial_y f + \hat{n}_z \partial_z f, \\ \partial_R^2 f &= \delta^{ik} \delta^{jl} n_i n_j \partial_k \partial_l f. \end{aligned} \quad (30)$$

B. Areal radius

Different options are available to define the areal radius coordinate from the $(3+1)$ -metric at the extraction sphere. A first choice, which we simply call the *areal radius*, is to consider the area of the two-dimensional manifold endowed with metric $\gamma_{ab} \equiv (\gamma_{\theta\theta}, \gamma_{\theta\phi}, \gamma_{\phi\phi})$,

$$r_{\text{areal}}^2 = \frac{1}{4\pi} \int \sqrt{\gamma_{\theta\theta}\gamma_{\phi\phi} - \gamma_{\theta\phi}^2} d\theta d\phi. \quad (31)$$

The expression assumes the manifold has the topology of a sphere. Since this is not guaranteed, the argument of the square root can become negative. Alternatively, Abrahams and Price [11] suggest considering just the diagonal component of the metric in the squared root above, which we call the *areal simple*. Note, however, that this choice sets to zero terms $(\partial_R \gamma_{\theta\phi})^2$ in the Hessian [see later Eq. (37b)]. Consequently, the even-parity master function $\Psi^{(e)}$ calculation gives unphysical amplitude already for a Schwarzschild background.

A second choice is the *average Schwarzschild* radius defined by Camarda and Seidel [12], which we motivate in detail. The “spherical part” of the 3-metric can be written as

$$\gamma_{ab} \equiv r^2 \sigma_{ab} + \sum_{\ell \geq 1} \sum_{m=-\ell}^{\ell} \alpha_{\ell m} Y_{ab}^{\ell m}, \quad (32)$$

where σ_{ab} is the 2-sphere metric (Appendix A) and the coefficients $\alpha_{\ell m}$ are functions of the radius r . The average Schwarzschild radius is found by integrating on the

2-sphere and using $\sigma_{ab}\sigma^{ab} = 2$ and orthogonality relations,

$$r_{\text{avg}}^2 = \frac{1}{8\pi} \int \left(\gamma_{\theta\theta} + \frac{\gamma_{\phi\phi}}{\sin^2 \theta} \right) d\Omega. \quad (33)$$

This choice give rise to two other obvious options, which are each of the terms contained in the expression above. We call them $g_{\theta\theta}$ and $g_{\phi\phi}$:

$$r_{g_{\theta\theta}}^2 = \frac{1}{4\pi} \int \gamma_{\theta\theta} d\Omega, \quad (34)$$

$$r_{g_{\phi\phi}}^2 = \frac{1}{4\pi} \int \frac{\gamma_{\phi\phi}}{\sin^2 \theta} d\Omega. \quad (35)$$

The performance of these choices will be tested for various spacetimes in Sec. IV.

Having identified the coordinate r , the 3-metric components on the extraction sphere, Eq. (29) are transformed to coordinates (t, r, θ, ϕ) ,

$$\begin{aligned} \beta_r &= \frac{\partial R}{\partial r} \beta_R, & \gamma_{rr} &= \frac{\partial R}{\partial r} \frac{\partial R}{\partial r} \gamma_{RR}, \\ \gamma_{r\theta} &= \frac{\partial R}{\partial r} \gamma_{R\theta}, & \gamma_{r\phi} &= \frac{\partial R}{\partial r} \gamma_{R\phi}, \end{aligned} \quad (36a)$$

together with the spatial derivatives,

$$\begin{aligned} \partial_r^{(4)} g_{00} &= \frac{\partial R}{\partial r} \partial_R^{(4)} g_{00}, & \partial_r \beta_r &= \frac{\partial^2 R}{\partial r^2} \beta_R + \left(\frac{\partial R}{\partial r} \right)^2 \partial_R \beta_R, \\ \partial_r \gamma_{rr} &= 2 \left(\frac{\partial R}{\partial r} \right) \frac{\partial^2 R}{\partial r^2} \gamma_{RR} + \left(\frac{\partial R}{\partial r} \right)^3 \partial_R \gamma_{RR}, \end{aligned} \quad (36b)$$

and the time derivatives

$$\begin{aligned} \partial_t \beta_r &= \partial_t \left(\frac{\partial R}{\partial r} \right) \beta_r + \frac{\partial R}{\partial r} \partial_t \beta_R \\ \partial_t \gamma_{rr} &= \left(\frac{\partial R}{\partial r} \right)^2 \left[-2 \frac{\partial R}{\partial r} \partial_t \left(\frac{\partial R}{\partial r} \right) \gamma_{RR} + \partial_t \gamma_{RR} \right], \\ \partial_t \gamma_{r\theta} &= \partial_t \left(\frac{\partial R}{\partial r} \right) \gamma_{R\theta} + \frac{\partial R}{\partial r} \partial_t \gamma_{R\theta}. \end{aligned} \quad (36c)$$

The above transformations require the inverse Jacobian and Hessian of the $r(R)$ transformation as well as to keep track of the time dependence in r . We illustrate these calculations for the average Schwarzschild radius (for which we drop the label hereafter); similar ones are performed for the other definitions of r . From Eq. (33), one gets

$$\frac{\partial r}{\partial R} = \frac{1}{16\pi r} \int \left(\partial_R \gamma_{\theta\theta} + \frac{\partial_R \gamma_{\phi\phi}}{\sin^2 \theta} \right) d\Omega \quad (37a)$$

$$\frac{\partial^2 r}{\partial R^2} = -\frac{1}{r} \left(\frac{\partial r}{\partial R} \right)^2 + \frac{1}{16\pi r} \int \left(\partial_R^2 \gamma_{\theta\theta} + \frac{\partial_R^2 \gamma_{\phi\phi}}{\sin^2 \theta} \right) d\Omega. \quad (37b)$$

and thus

$$\frac{\partial^2 R}{\partial r^2} = - \left(\frac{\partial R}{\partial r} \right)^3 \frac{\partial^2 r}{\partial R^2}. \quad (37c)$$

For the time derivatives, one computes

$$\partial_t \left(\frac{\partial r}{\partial R} \right) = -\frac{\dot{r}}{r} \frac{\partial r}{\partial R} + \frac{1}{16\pi r} \int \left(\partial_t \partial_R \gamma_{\theta\theta} + \frac{\partial_t \partial_R \gamma_{\phi\phi}}{\sin^2 \theta} \right) d\Omega, \quad (37d)$$

and thus

$$\partial_t \left(\frac{\partial R}{\partial r} \right) = - \left(\frac{\partial R}{\partial r} \right)^2 \partial_t \left(\frac{\partial r}{\partial R} \right). \quad (37e)$$

The derivatives of $r(t)$ are

$$\dot{r} = \frac{1}{16\pi r} \int \left(\partial_t \gamma_{\theta\theta} + \frac{\partial_t \gamma_{\phi\phi}}{\sin^2 \theta} \right) d\Omega \quad (37f)$$

$$\ddot{r} = -\frac{(\dot{r})^2}{r} + \frac{1}{16\pi r} \int \left(\partial_t^2 \gamma_{\theta\theta} + \frac{\partial_t^2 \gamma_{\phi\phi}}{\sin^2 \theta} \right) d\Omega. \quad (37g)$$

C. Background 2-metric

Given the $(3+1)$ -metric in spherical coordinates (t, r, θ, ϕ) at the extraction sphere, the background 2-metric is computed by averaging on the sphere, i.e., extracting the monopoles:

$$g_{00} = -\frac{1}{4\pi} \int (\alpha^2 - \beta_i \beta^i) d\Omega, \quad (38a)$$

$$g_{01} = \frac{1}{4\pi} \int \beta_r d\Omega, \quad (38b)$$

$$g_{11} = \frac{1}{4\pi} \int \gamma_{rr} d\Omega. \quad (38c)$$

D. Projection of $(3+1)$ -metric

Given the $(3+1)$ -metric and the background 2-metric in coordinates (t, r, θ, ϕ) , it is possible to compute the multipoles at the extraction sphere. The even-parity multipoles in Eq. (3) are computed from the projections

$$h_{00}^{(\ell m)} = - \int (\alpha^2 - \beta_i \beta^i) Y_{\ell m}^* d\Omega, \quad (39a)$$

$$h_{01}^{(\ell m)} = \int \beta_r Y_{\ell m}^* d\Omega, \quad (39b)$$

$$h_{11}^{(\ell m)} = \int \gamma_{rr} Y_{\ell m}^* d\Omega \quad (39c)$$

$$h_0^{(\ell m)} = \frac{1}{\lambda} \int \left(\beta_\theta \partial_\theta Y_{\ell m}^* + \frac{\beta_\phi}{\sin^2 \theta} \partial_\phi Y_{\ell m}^* \right) d\Omega, \quad (39d)$$

$$h_1^{(\ell m)} = \frac{1}{\lambda} \int \left(\gamma_{r\theta} \partial_\theta Y_{\ell m}^* + \frac{\gamma_{r\phi}}{\sin^2 \theta} \partial_\phi Y_{\ell m}^* \right) d\Omega, \quad (39e)$$

$$K_{\text{RW}}^{(\ell m)} = \frac{1}{2r^2} \int \left(\gamma_{\theta\theta} + \frac{\gamma_{\phi\phi}}{\sin^2 \theta} \right) Y_{\ell m}^* d\Omega + \frac{1}{2r^2(\lambda - 2)} \int \left[\left(\gamma_{\theta\theta} - \frac{\gamma_{\phi\phi}}{\sin^2 \theta} \right) W_{\ell m}^* + \frac{2}{\sin^2 \theta} \gamma_{\theta\phi} X_{\ell m}^* \right] d\Omega, \quad (39f)$$

$$G^{(\ell m)} = \frac{1}{r^2 \lambda (\lambda - 2)} \int \left[\left(\gamma_{\theta\theta} - \frac{\gamma_{\phi\phi}}{\sin^2 \theta} \right) W_{\ell m}^* + \frac{2}{\sin^2 \theta} \gamma_{\theta\phi} X_{\ell m}^* \right] d\Omega, \quad (39g)$$

where we have defined the functions [2]

$$\begin{aligned} W_{\ell m} &:= \frac{1}{\sin \theta} \nabla_{(\phi} S_{\theta)}^{(\ell m)} \\ &= \partial_\theta^2 Y_{\ell m} - \cot \theta \partial_\theta Y_{\ell m} - \frac{1}{\sin^2 \theta} \partial_\phi^2 Y_{\ell m} \\ &= (2\partial_\theta^2 + \lambda) Y_{\ell m}, \end{aligned} \quad (40a)$$

$$\begin{aligned} X_{\ell m} &:= -\sin \theta \left(\nabla_\theta S_\phi^{(\ell m)} - \frac{\nabla_\phi S_\theta^{(\ell m)}}{\sin^2 \theta} \right) \\ &= 2(\partial_{\theta\phi}^2 Y_{\ell m} - \cot \theta \partial_\phi Y_{\ell m}). \end{aligned} \quad (40b)$$

The odd-parity multipoles in Eq. (5) are computed from the following projections:

$$H_0^{(\ell m)} = \frac{1}{\lambda} \int \frac{1}{\sin \theta} (-\beta_\theta \partial_\phi Y_{\ell m}^* + \beta_\phi \partial_\theta Y_{\ell m}^*) d\Omega, \quad (41a)$$

$$H_1^{(\ell m)} = \frac{1}{\lambda} \int \frac{1}{\sin \theta} (-\gamma_{r\theta} \partial_\phi Y_{\ell m}^* + \gamma_{r\phi} \partial_\theta Y_{\ell m}^*) d\Omega, \quad (41b)$$

$$\begin{aligned} H^{(\ell m)} &= \frac{1}{\lambda(\lambda - 2)} \int \left[\frac{1}{\sin \theta} \left(-\gamma_{\theta\theta} + \frac{\gamma_{\phi\phi}}{\sin^2 \theta} \right) X_{\ell m}^* \right. \\ &\quad \left. + \frac{2\gamma_{\theta\phi}}{\sin \theta} W_{\ell m}^* \right] d\Omega. \end{aligned} \quad (41c)$$

Similar projections are performed on the time and radial derivatives of the $(3 + 1)$ -metric in order to obtain time and radial derivatives of the multipoles. The latter are required to construct the master functions in Eqs. (15), (19), (20), (22), and (25). Note that we do *not* subtract the background metric. Although this may improve the multipole computation in simulations at low resolutions, we rely exclusively on the orthogonality of spherical harmonics for the projections.

IV. SIMULATIONS

We implement the above algorithm in GR-Athena++ [61–63]. GR-Athena++ implements modules for solving the Z4c free-evolution scheme of Einstein equations [64,65]

coupled to radiation magnetohydrodynamics equations in Eulerian $(3 + 1)$ conservative formulation. In this work, we consider simulations involving only hydrodynamics and metric evolution; for the gauge sector, we adopt the moving puncture gauge implemented as described in Ref. [61].

GR-Athena++ uses a Cartesian mesh and a block-based adaptive mesh refinement (AMR) strategy, in which the computational domain is divided into mesh block (MB). The MBs can be individually refined, splitting into (in three dimensions) eight new MBs with double linear resolution. Each MB exists on a single refinement level. Our simulations are performed in three dimensions without symmetries. Therefore, the grid is defined by the number of points along each dimension for the coarsest level N_M ; the number of refinement levels $0, \dots, N_L$; and the number of points along each dimension in the MB. The latter is fixed to $N_B = 16$ for all problems. We use the cell-centered representation for spacetime variables and, for binary problems, the AMR criterion described by Rashti *et al.* [66] (L_2 -norm based, used for black hole cases) and Daszuta *et al.* [63] (L_∞ -norm based, used for matter cases).

Metric variables are discretized using finite differencing operators of fourth-order accuracy for problems involving neutron stars and sixth-order accuracy for problems with binary black holes. Kreiss-Oliger dissipation operators are utilized to suppress numerical noise with parameter σ . Finite volume (high-resolution shock capturing) methods based on the local Lax-Friedrichs flux and weighted essentially non-oscillatory (Z version) reconstruction are used for the discretization of hydrodynamics equations following closely Ref. [62]. Time integration of all equations is performed explicitly via the method of lines, using a low storage fourth-order Runge-Kutta with fixed time step across all levels and subject to a Courant-Friedrich-Lewy (CFL) condition.

Gravitational waves are extracted at coordinate spheres. GR-Athena++ implements both spherical geodesic grids and latitude-longitude spheres. The former are employed for the extraction of the Weyl ψ_4 pseudoscalar using a resolution of 9002 vertices ($n_Q = 30$) [61]. The latter are used for the RWZ extraction. Output for CCE is also dumped at the

same spheres. Waveforms and other quantities are shown as a function of the retarded time $u = t - r_*$, where $r_* = r_*(r(R))$ is the tortoise coordinate associated to the isotropic radius of the extraction sphere and the Arnowitt-Deser-Misner (ADM) mass of the spacetime is employed in the transformation.

The latitude-longitude grids for the RWZ extraction are evenly spaced in the longitude coordinate ϕ , while we use Gauss-Legendre nodes for the coordinate θ . For the simulations presented here, we choose $N_\theta = N_\phi/2 = 128$ nodes in each direction in order to obtain good-quality waveforms for all the different problems considered at a sufficiently large extraction distance. Integrals on the 2-sphere are computed with Gauss-Legendre quadratures; other details are given in Appendix B. CCE waveforms are computed using the `PitNull` code [44,67]. These CCE data are in terms of Weyl's pseudoscalar or News function and thus require integration to compute the RWZ multipoles. The strain multipoles from both ψ_4 multipoles and the CCE News multipoles is calculated using both the fixed frequency integration (FFI) [30] method, or the direct time integration (DTI), e.g., Refs. [15,68]. The former method requires the identification of a cutting frequency f_0 for the high-pass filters applied during the frequency-domain integration. The latter method introduces a drift in the integrated multipole that requires a polynomial corrections. These choices are detailed and discussed below for each problem considered.

The mesh setups in this work are specified by prescribing a base cubic grid $\Omega = [x_{\min}, x_{\max}]^3$ (refinement level zero) covered by N_M points per direction and with resolution $h_0 = (x_{\max} - x_{\min})/N_M$ in each direction. N_L static or adaptive mesh refinements are added from the beginning of the simulation; the highest resolution is achieved at the highest refinement level, h_L . Table II summarizes the GR-Athena++ setup for all the problems discussed in this work. The simulated spacetimes are Tolman-Oppenheimer-Volkoff (TOV) (static and spherically symmetric) stars with a fluid or spacetime perturbation, gravitational collapse of a rotating neutron star (RNS), binary black hole (BBH) circular merger and dynamical capture, and a binary neutron star (BNS) circular merger.

V. PERTURBED TOV SPACETIMES

In a first test of the extraction algorithm, we consider the evolution of a TOV star which is perturbed in either the even or the odd sector using a fluid or a spacetime perturbation, respectively. The initial perturbation excites the star's proper modes and the emission of GWs. We compare systematically waveforms computed with the metric extraction algorithm to those from the NP algorithm and CCE waveforms. The initial data coordinates are Schwarzschild isotropic coordinates, and the puncture gauge keeps the coordinates very close to the initial ones during the evolution. Therefore, this test also allows us to probe the consistency of the different RWZ master functions in the scenario of a static background in known coordinates.

The GR-Athena++ setup for this test is as follows (see also Table II). The refinement level zero covers the domain $\Omega = [-512M_\odot, 512M_\odot]^3$ with $N_M = (64, 96, 128)$ points per direction. Six static mesh refinement levels are employed to resolve the star up to a maximum resolution $h_6 = 0.125M_\odot$ over the entire star. The CFL factor is set to 0.25, and the Kreiss-Oliger dissipation parameter is $\sigma = 0.5$. The extraction spheres for the RWZ and NP algorithms are located at $R = (75, 100, 150, 200, 250, 300, 350, 400, 450)M_\odot$, while the world-tube output for the CCE is dumped at $R = (150, 250, 350, 450)M_\odot$.

A. Even-parity perturbations

We consider a TOV star of gravitational mass $M_{\text{TOV}} = 1.36M_\odot$ and whose matter is described by the piecewise polytropic fit to the SLy equation of state (EOS) [69]. The isotropic radius of the star is $R_{\text{TOV}} = 7.76M_\odot$. Even-parity modes are excited by superimposing an axisymmetric pressure perturbation to the initial TOV data [15],

$$\delta p(R, \theta) = (p + e)A \sin\left(\frac{\pi R}{2R_{\text{TOV}}}\right) Y_{\ell 0}(\theta), \quad (42)$$

where p (e) is the TOV pressure (energy density) and we choose $A = 0.005$ and $\ell = 2$.

The GWs from these simulations are approximately monochromatic signals of frequencies corresponding to

TABLE II. Simulations setup. For each problem, the columns report: the extension of refinement level zero Ω (lengths are in units of $M_\odot$), the number of points per direction N_M , the number of refinement levels N_L , the wave-extraction radii R (only where the CCE data is dumped, in which all the algorithms can be compared), the corresponding resolution at the extraction radii δR , the CFL factor, and the Kreiss-Oliger dissipation parameter σ .

Problem	Ω	N_M	N_L	R ($M_\odot$)	δR ($M_\odot$)	CFL	σ
TOV	$[-512, 512]^3$	64, 96, 128	6	150, 250, 350, 450	4, 4, 8, 8	0.25	0.5
RNS	$[-512, 512]^3$	96, 128, 192	7	150, 250, 350, 450	5.33, 5.33, 5.33, 5.33	0.2	0.1
BBH	$[-1536, 1536]^3$	128, 192	10	100, 140, 220, 400	2, 2, 4, 8	0.25	0.2
BNS	$[-1024, 1024]^3$	160	6	200, 400, 600, 800	3.2, 6.4, 12.8, 12.8	0.25	0.5

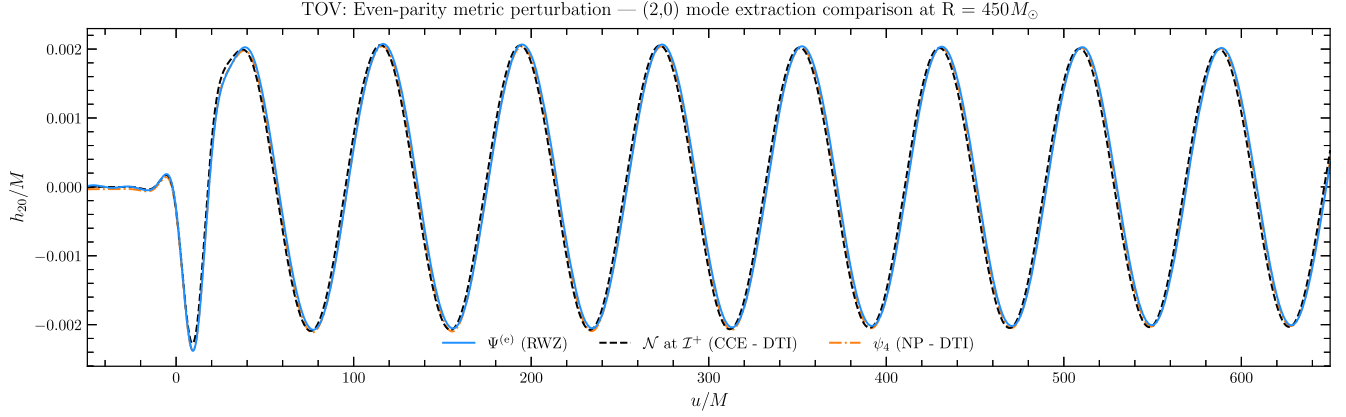


FIG. 1. Strain (2, 0) mode for the TOV problem with pressure perturbation [Eq. (42)] extracted at $R = 450M_\odot$. Different lines refer to different extraction algorithms: RWZ (solid blue), CCE (dashed black), and NP (dot-dashed orange). The mode is dominated by the f -mode frequency of the star. Data refer to the highest resolution simulation.

the f -modes excitations. Figure 1 shows the dominant (2, 0) mode of the strain as computed from RWZ and NP multipoles extracted at $R = 450M_\odot$ and compared to CCE data evolved from the same extraction radius. Throughout this paper, we will represent the dynamical background in general coordinates RWZ wave in solid blue, the CCE in dashed black, and the NP in dot-dashed orange. The figure shows good agreement between the different extraction methods; CCE waveforms are slightly dephased with respect to finite extraction. This dephasing increases at smaller extraction radii (not shown) and fixed resolution. We mention that, due to quasimonochromatic character of the signal, the strain from the ψ_4 and CCE News waveforms can be obtained using both the FFI (with $f_0 \lesssim f$) and DTI method. In the following, we only consider DTI integrated waveforms using a linear polynomial subtraction applied to the entire signal.

We first demonstrate convergence of the RWZ waveform by considering simulations with $N_M = 64, 96, 128$ points which correspond to a maximal resolutions $h_6 = 0.25, 0.167, 0.125M_\odot$. The three meshes are indicated as LR, MR, and HR. Focusing on the (2, 0) RWZ $\Psi^{(e)}$ mode, the differences of data from simulations at successive resolutions are shown in Fig. 2. The plot also shows the differences MR-HR rescaled by the appropriate factor for second-order convergence. Waveforms at all extraction radii show consistent second-order convergence, compatible with the truncation error of hydrodynamics.

Finite-radius extraction effects on the waveform amplitude are summarized in Fig. 3, which shows the 10th amplitude peak of waveforms as function of the inverse extraction radii. The peak amplitude converges to the CCE peak the larger the extraction radius is and for both RWZ and NP multipoles. The maximum amplitude differences remain below the 2% in the range $R \in [150, 450]M_\odot$ for all extraction algorithms. The RWZ multipole shows larger deviations from CCE than the NP multipole, but such deviations are smaller than mesh resolution effects.

Inspection of the full waveform indicates that the best extraction radius is the largest considered, at which data from the various algorithm are most compatible with each other.

TOV: Even-parity pressure perturbation — RWZ convergence test using $N_M = 64, 96, 128$

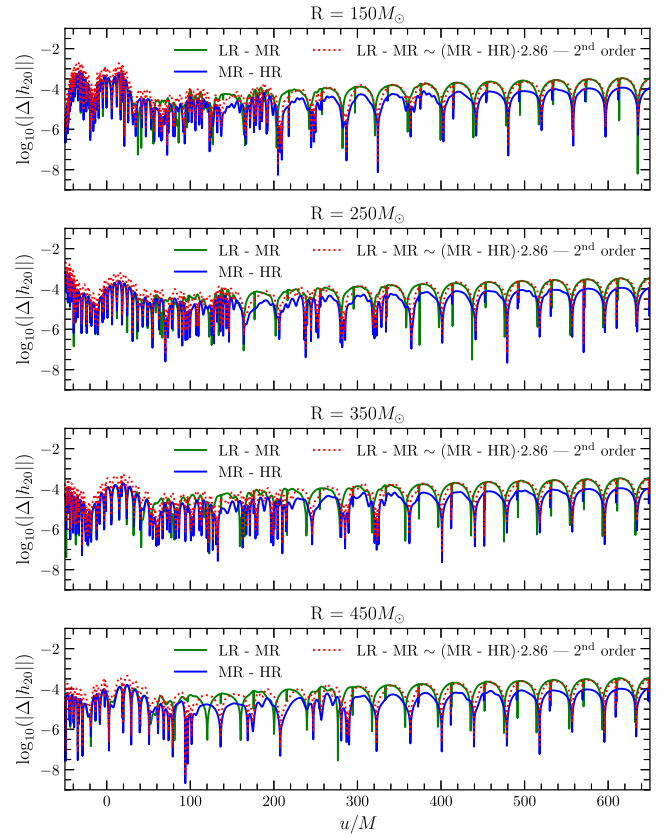


FIG. 2. Convergence test of the RWZ (2, 0) mode for the TOV problem with pressure perturbation [Eq. (42)]. Different solid lines refer to differences between data from simulations at successive resolutions $N_M = 64, 96, 128$ labelled LR, MR, and HR. The dotted red line is the blue line rescaled by second-order convergence. Different panels show representative extraction radii.

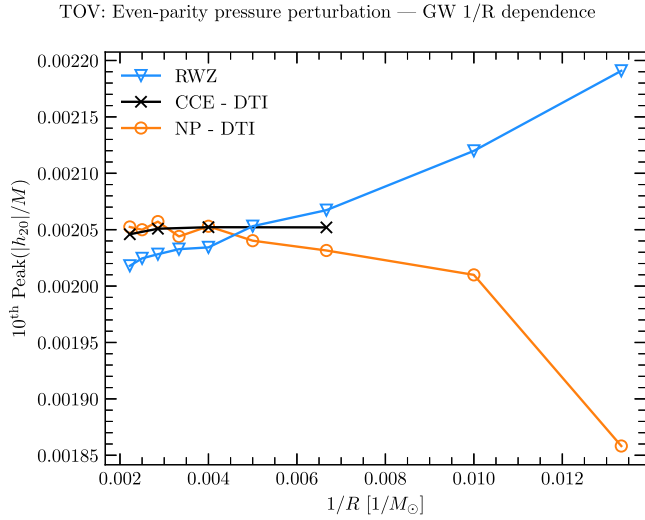


FIG. 3. Extraction radius dependence of the amplitude's 10th peak of the strain (2, 0) mode for the TOV problem with pressure perturbation [Eq. (42)]. Different lines refer to different extraction algorithms: RWZ (blue), CCE (black), and NP (orange). The dotted gray vertical line marks the radius with the best overall compatibility. Data refer to the highest-resolution simulation.

We compare the RWZ different even-parity master functions $\Psi_{20}^{(e)}$ [Eq. (20), blue], $\Psi_{\text{static } 20}^{(e)}$ [Eq. (19), dot-dashed light green], and Q_{+20} [Eq. (15) normalized as per Eq. (21), dotted dark green] in Fig. 4. Relative amplitude differences with respect to $\Psi^{(e)}$ are around 10^{-5} for both $\Psi_{\text{static}}^{(e)}$ and Q_+ . This sets the level of consistency of three methods up to truncation errors for a static background. The bottom panel of Fig. 4 also shows the amplitude relative differences in $\Psi^{(e)}$ due to different choices for the Schwarzschild radius used to build the background for the master functions. The different choices are tested by running otherwise identical simulations at resolution $N_M = 128$. The areal and average Schwarzschild radius definitions provide waveforms compatible to $\lesssim 10^{-5}$ level, while the $g\theta\theta$ and $g\phi\phi$ choices (compatible with each other) introduce larger differences. These differences originate from numerical errors in the different integral expressions for the Schwarzschild radius (see below). The choice of Schwarzschild radius is anyway an uncertainty significantly smaller than the choice of extraction algorithm and of the extraction radii.

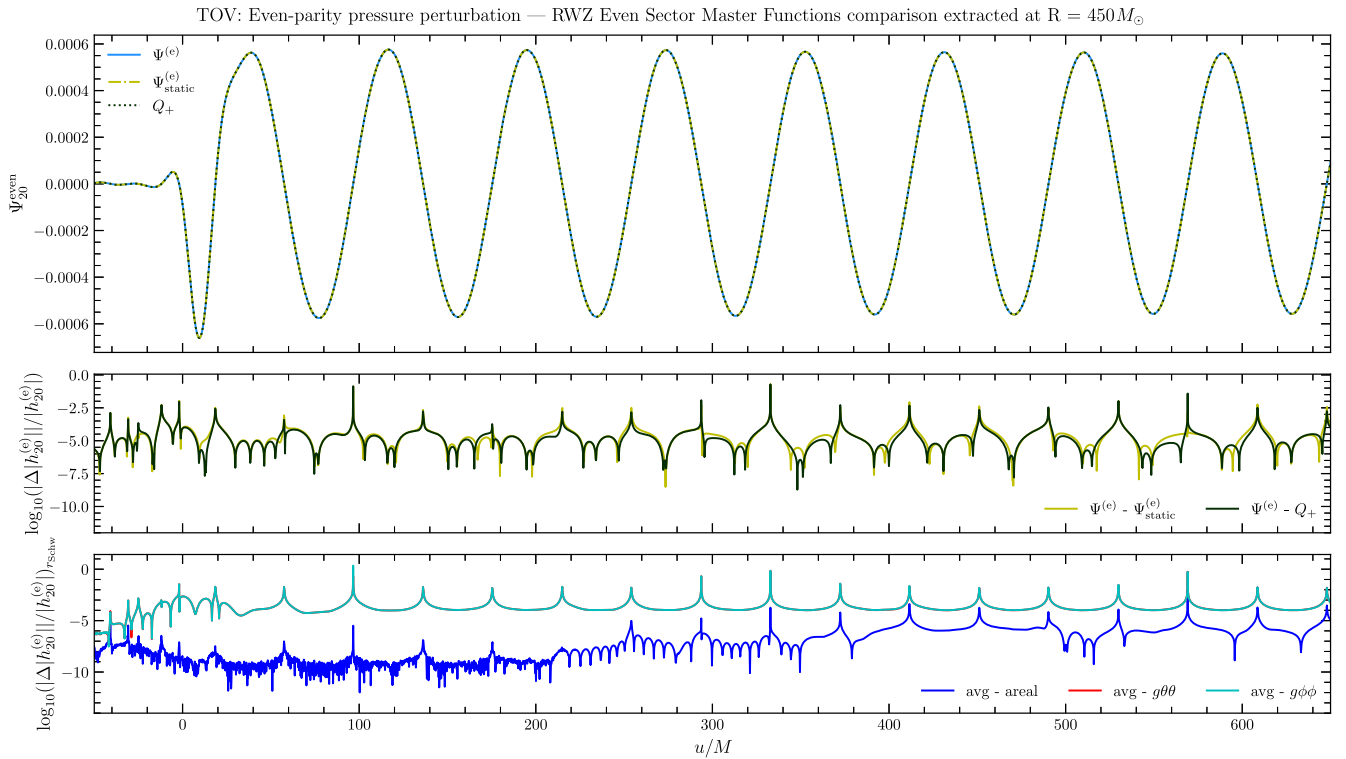


FIG. 4. RWZ (2, 0) mode for the TOV problem with pressure perturbation [Eq. (42)] extracted at $R = 450M_\odot$ computed using different RWZ master functions. Top: even-parity master function extraction comparison $\Psi^{(e)}$ (solid blue), $\Psi_{\text{static}}^{(e)}$ (dot-dashed light green), and Q_+ (dotted dark green) normalized as per Eq. (21). Middle: amplitude relative differences with respect to $\Psi^{(e)}$. Bottom: $\Psi^{(e)}$ amplitude relative differences with respect to different choices of the Schwarzschild radius definitions with respect to the average Schwarzschild radius choice. Data refer to the highest-resolution simulation.

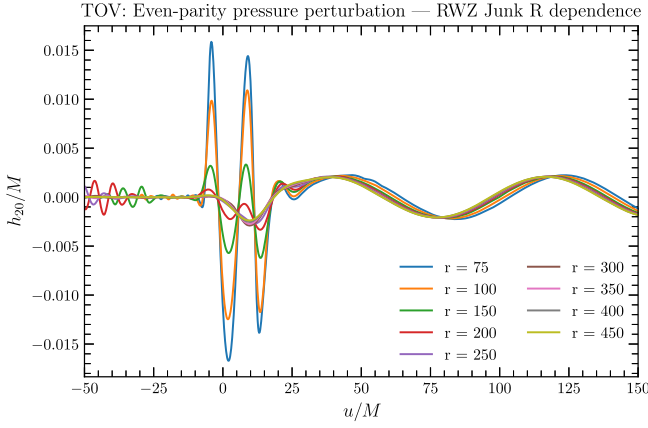


FIG. 5. Strain (2, 0) mode for the TOV problem with pressure perturbation [Eq. (42)] extracted at different radii (in units of $M_\odot$) close to the initial junk radiation.

Baiotti *et al.* [15] reported that junk radiation in RWZ waveforms from perturbed TOV can unphysically increase with the extraction radius. They argue that numerical uncertainties are a possible cause of this behavior; see their Fig. 13 and the related discussion. As demonstrated by Fig. 5, we do not observe such an issue in our implementation: the junk radiation converges with the radius of the extraction sphere. The main numerical improvements in our algorithm are the interpolation to the extraction sphere (here performed at high order) and the computation of the projections using Gauss-Legendre quadrature, see Appendix B.

Finally, the TOV spacetime simulations allow us to investigate the numerical computation of the spherical background in the metric extraction algorithm. In particular, we consider a comparison of the estimated Schwarzschild mass given by Eq. (A8) with the TOV mass M_{TOV} and of the analytical Schwarzschild radius

$$r = R \left(1 + \frac{M_{\text{TOV}}}{2R} \right)^2, \quad (43)$$

with the possible choices discussed above. The left panels of Fig. 6 show that both the mass and the Schwarzschild radius are affected by uncertainties of order $\lesssim 10^{-4}$. The uncertainties decrease with larger extraction radii. The right panels of Fig. 6 show differences in the mass and Schwarzschild radius introduced by different choices of the latter in the metric extraction algorithm. The average Schwarzschild, areal, and areal-simple prescriptions provide practically identical results and perform better than the $g\theta\theta$ and $g\phi\phi$ prescriptions. The latter two show deviation up to a few percent.

B. Odd-parity perturbations

We consider a TOV star described by SLy EOS and with gravitational mass $M_{\text{TOV}} = 2M_\odot$ and isotropic radius $R_{\text{TOV}} = 7.22M_\odot$. Odd-parity modes are excited by superposing a metric perturbation,

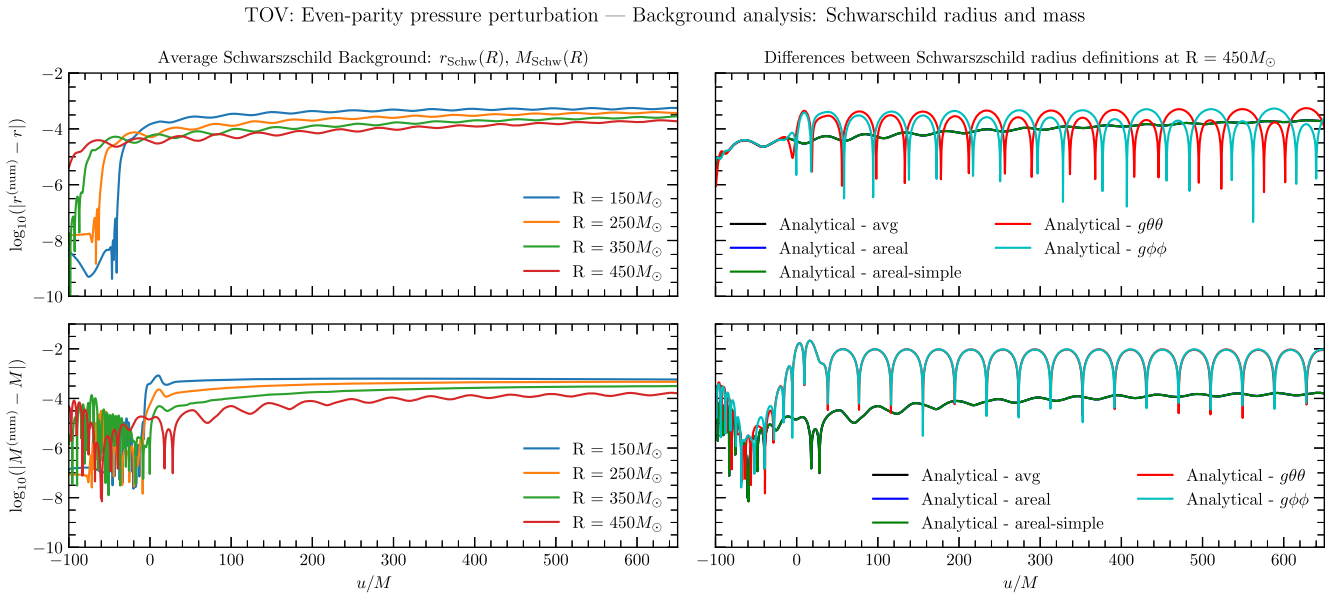


FIG. 6. Background mass and Schwarzschild radius computation in the TOV problem with pressure perturbation [Eq. (42)]. Left: differences between the analytical and numerical background Schwarzschild radius (top) and mass (bottom) as a function of retarded time and different isotropic extraction radii R . The average Schwarzschild radius is employed in this simulation. Right: different lines show the same differences as the left panels but compare simulations with different choices for the Schwarzschild radius. Data are compared at $R = 450M_\odot$. All data refer to the highest-resolution simulation.

$$\delta g_{\mu\nu} = \Phi(R) \Re \left(\begin{array}{c|cc} 0 & 0 & 0 \\ \hline & S_{\theta}^{(\ell,m)} & S_{\phi}^{(\ell,m)} \\ 0 & S_{\theta}^{(\ell,m)} & 0 \\ \hline 0 & S_{\phi}^{(\ell,m)} & 0 \end{array} \right), \quad (44)$$

similarly as in the work by Pazos *et al.* [13]. We choose a Gaussian pulse

$$\Phi(R) = A e^{-\left(\frac{R-10R_{\text{TOV}}}{0.15R_{\text{TOV}}}\right)^2}. \quad (45)$$

with $A = 0.0001$ and a $(\ell, m) = (2, 0)$ perturbation which makes $\delta g_{r\phi}$ be the only nonvanishing component. The initial perturbation scatters against the star and excites the w -modes of the star [70]. In this case, we enforce the shift to be 0 during the evolution to avoid spurious signals in some modes due to gauge effects.

The dominant GW strain mode $(2, 0)$ from these simulations is shown in Fig. 7; it is computed from RWZ and NP

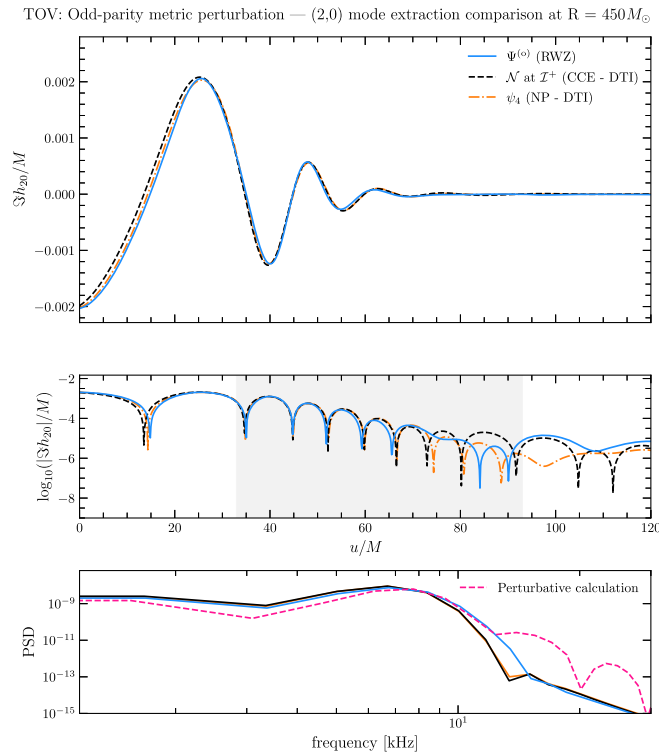


FIG. 7. Strain $(2, 0)$ mode for the TOV problem with spacetime perturbation [Eq. (44)] extracted at $R = 450M_{\odot}$. Top: different lines refer to different extraction algorithms: RWZ (solid blue), CCE (dashed black), and NP (dot-dashed orange). The mode is dominated by the w -mode frequency of the star. Middle: same as top panel but in logarithmic scale. Bottom: PSD of the shaded area in the middle panel (ringdown part) and comparison to perturbative results (dashed pink). Data refer to the highest-resolution simulation.

multipoles extracted at $R = 450M_{\odot}$ and compared to CCE data evolved from the same extraction radius. For the integration of the ψ_4 and News function, we experimented with both FFI ($f_0 = 0.002/M$) and DTI to find robust results; we again discuss results for the DTI method with a linear polynomial subtraction.

The RWZ extraction is found to be overall compatible with CCE and NP. CCE data show again a small and convergent dephasing with respect to the finite extraction waveforms. The largest quantitative differences are found in the ringdown at late times $u/M \sim 65 - 90$ (middle panel). The bottom panel show the power spectral density (PSD) of the ringdown part of the signal (shaded area from the center panel). The PSD is compared to a perturbative simulation obtained using the $(1+1)$ -dimensional $[(1+1)\text{D}]$ code PerBACC0 [71]. Note the latter code employs a slightly different initial condition (perturbation) than Eq. (44). Nonetheless, the ringdown spectra are in good agreement, and the w -mode perturbative peak frequency at ~ 7749 Hz is compatible with the three-dimensional (3D) numerical relativity simulation. To our knowledge this is the first experiment obtaining w -modes in a 3D simulations without symmetries; previous work has considered octant symmetry and inverse Cowling approximation [72].

We compare the different $(2, 0)$ RWZ odd-parity master functions in Fig. 8. The relative differences between $\Psi^{(o)}$ and $\Psi_{\text{static}}^{(o)}$ show very good consistency between the two calculations. They are around 5 orders of magnitude smaller than in the even-parity case. This pattern appears to be consistent among all of the simulation considered, as discussed also below. Relative differences between $\Psi^{(o)}$ and $Q_{\times}$ are instead significantly larger. We attribute this

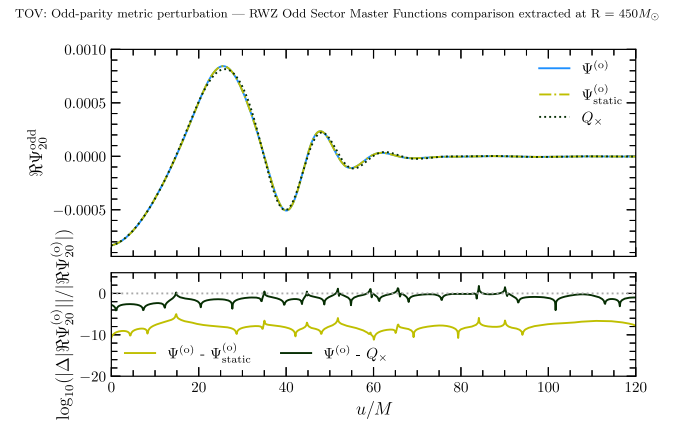


FIG. 8. RWZ $(2, 0)$ mode for the TOV problem with spacetime perturbation [Eq. (44)] extracted at $R = 450M_{\odot}$. Top: odd-parity master function extraction comparison $\Psi^{(o)}$ (solid blue), $\Psi_{\text{static}}^{(o)}$ (dot-dashed light green), and $Q_{\times}$ (dotted dark green) integrated and normalized as per Eq. (27). Bottom: amplitude relative differences with respect to $\Psi^{(o)}$. Data refer to extraction radius $R = 450M_{\odot}$ and the highest-resolution simulation.

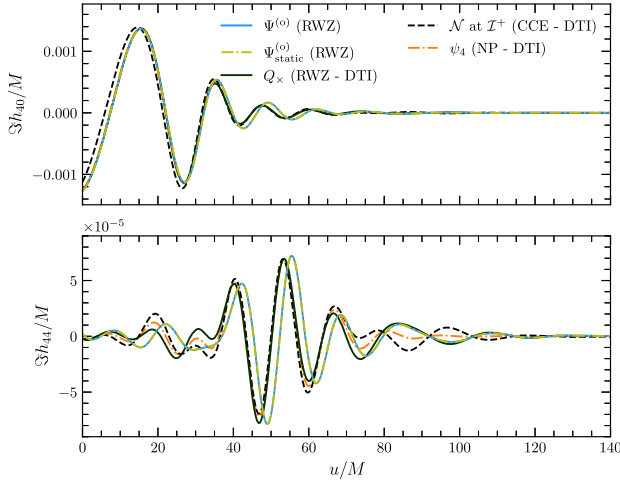
TOV: Odd-parity metric perturbation — (4,0), (4,4) modes extraction comparison at $R = 450M_\odot$ 

FIG. 9. Strain higher modes for the TOV problem with spacetime perturbation [Eq. (44)] extracted at $R = 450M_\odot$. Different lines refer to different extraction algorithms: RWZ $\Psi^{(o)}$ (solid blue), CCE (dashed black), NP (dot-dashed orange), RWZ $\Psi^{(o)}_{\text{static}}$ (dot-dashed light green), and the time integrated/normalized of $Q_\times$ (dotted dark green) signals. The top (bottom) panel refers to the (4, 0) [(4, 4)] mode. Data refer to extraction radius $R = 450M_\odot$ and the highest-resolution simulation.

fact to the time integration required to match the RWZ $\Psi^{(o)}$ normalization, as per Eq. (27).

Finally, we provide a waveform comparison of the first subdominant modes in Fig. 9. The first nonzero mode is the (4, 0): it has an amplitude about a factor 2 smaller than the dominant (2, 0) mode and a ringdown part qualitatively very similar to the (2, 0). All extraction algorithms deliver consistent waveforms, with CCE data showing a dephasing at early times. This is, as above, related to the finite extraction of the RWZ and NP modes. Differences among extraction algorithms become more evident in the (4, 4) mode, which is about 3 orders of magnitude smaller than the (2, 0). The $\Psi^{(o)}$ and $\Psi^{(o)}_{\text{static}}$ extraction suffer from a larger dephasing with respect to $Q_\times$, possibly due to truncation errors propagating in the calculation of Eqs. (19) and (20) and affecting the small-amplitude signal. Interestingly, the $Q_\times$ master function nicely agrees with CCE and NP around the peak of the waveform.

VI. GRAVITATIONAL COLLAPSE OF A ROTATING NEUTRON STAR

We consider simulations of the gravitational collapse of a rotating neutron star to a black hole, e.g., Refs. [28,32,62,73]. Reisswig *et al.* [28] presented waveforms using a metric extraction algorithm based on Schwarzschild coordinates, i.e., Q_+ . Here, we consider for the first time also waveforms with the covariant and gauge-invariant metric algorithm.

The simulations use the same refinement level zero domain Ω as for the TOV problems but this time refined with $N_L = 7$ static refinement levels. The domain is resolved with $N_M = (96, 128, 192)$ points to achieve a maximal resolution of $h_7 = 0.0417M_\odot$. The CFL factor is set to 0.2, and the Kreiss-Oliger dissipation parameter is set to $\sigma = 0.1$. Gravitational waves are extracted at the same radii as for the TOV problems.

We consider the uniformly rotating D4 neutron star model already simulated in, e.g., Refs. [32,73] with gravitational mass $M = 1.86M_\odot$ and polar-to-equatorial coordinate axis ratio of $r_p/r_e = 0.65$. The rotation frequency is close to the Kepler limit, which sets the mass shedding and stability limit. Initial data for the simulation are generated with the RNS code [74]. We introduce a pressure perturbation in the initial data which decreases the star's pressure by 0.21 percent, uniformly over the pressure profile. This helps to accelerate the rotational collapse but delays collapse enough to clearly separate the junk radiation from the rest of the gravitational signal [32].

The GWs from the rotational collapse has the well-known *precursor-burst-ringdown* morphology [75], and it is entirely in the even-parity sector. The background spacetime is now dynamical and in coordinates defined by the 1 + log and Γ -driver evolution equation (gauge sector of the Z4c free-evolution scheme). Figure 10 shows the strain (2, 0) mode from the RWZ, CCE, and NP extractions

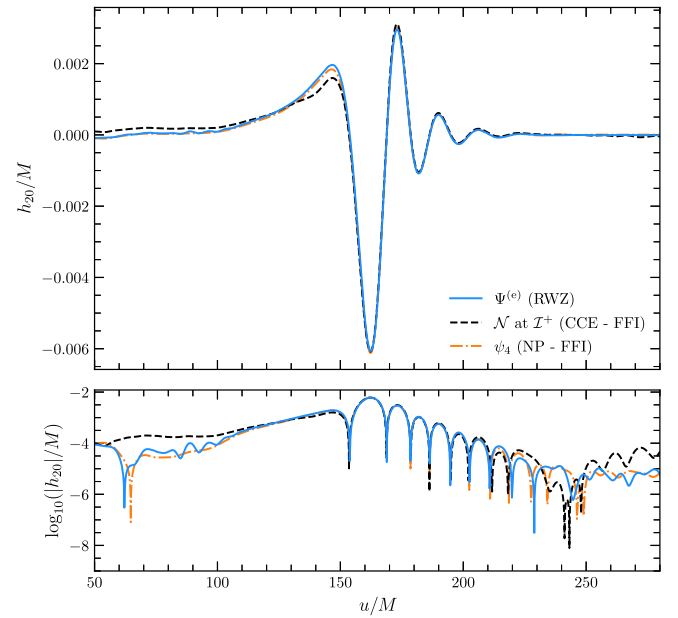
RNS Collapse: — (2,0) mode extraction comparison at $R = 450M_\odot$ 

FIG. 10. Strain (2, 0) mode for the rotating collapse problem extracted at $R = 450M_\odot$. Different lines refer to different extraction algorithms: RWZ (solid blue), CCE (dashed black), and NP (dot-dashed orange). The top (bottom) panel shows the waveform in linear (log) scale. Data refer to the highest-resolution simulation.

RNS Collapse — GW amplitude radial dependence

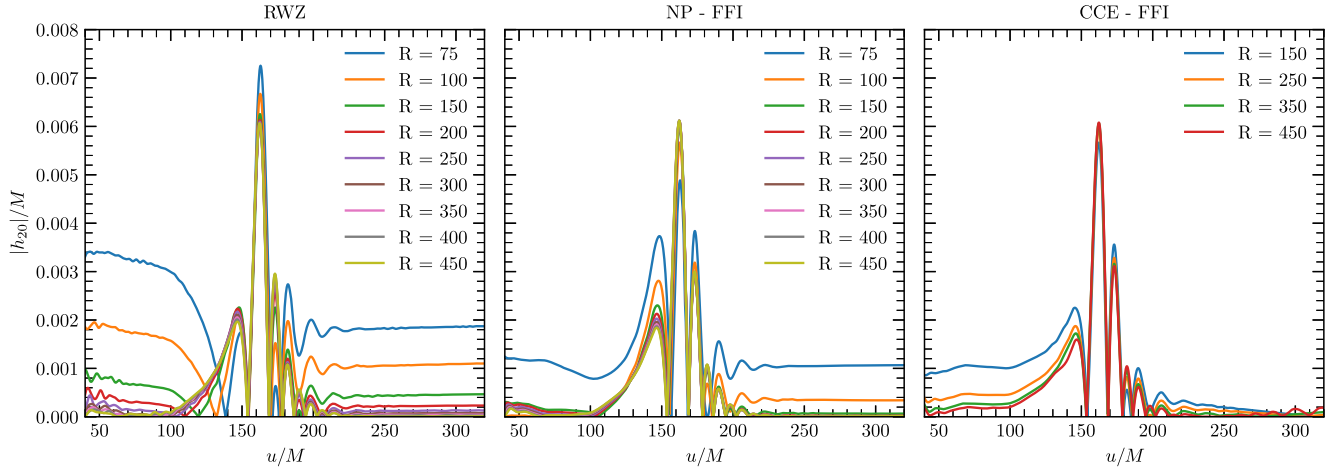


FIG. 11. Extraction radius dependence of the strain $(2, 0)$ mode for the rotating collapse problem. Panels from left to right: RWZ, NP, and CCE extraction. For each panel, different lines show different extraction radii (in units of $M_\odot$). Data refer to the highest-resolution simulation.

at $R = 450M_\odot$. The three methods deliver compatible waveforms with the expected morphology. The largest differences are visible at early times in the precursor and at late time in the ringdown. Starting from the latter, the lower panel shows that the ringdown oscillations are well captured until the ninth peak, $u/M \lesssim 240$. After that, the RWZ extraction first and then both CCE and NP become noisy due to the small amplitude of the signal. The differences in the precursor are due to two effects. On the one hand, the RWZ extraction gives more noisy waveforms than other methods, see the spurious oscillation around $u/M \sim 90$, which converges away with resolution. This is compatible with what is observed by Reisswig *et al.* [28]. On the other hand, the integration of the CCE ψ_4 or News function introduces here some uncertainty in the strain. In the absence of a physically motivated cutoff frequency, we experimented with both the FFI and the DTI integration. We find that the double integral of the CCE ψ_4 result in spurious oscillations with both methods, while the integral of the News shows unphysical drifts for various choices of the polynomial correction. These issues are not present in the ψ_4 extracted at finite radii. Best results are obtained using FFI with $f_0 = 0.00149/M$ and integrating the CCE News, which are shown in the figure.

The dependence of the waveforms on the extraction (or world-tube) radii is shown in Fig. 11. Significant finite extraction effects are evident at both early and late times for radii $R \lesssim 200M_\odot$ in the RWZ and NP methods. The peak of the RWZ waveform is clearly more sensitive to the choice of extraction sphere in this problem. Also, the precursor in the integrated CCE data is strongly dependent on the world-tube radii. However, waveforms converge to each other for radii $R \gtrsim 350M_\odot$. To better quantify this convergence, Fig. 12 shows the GW maximum amplitude (the GW burst)

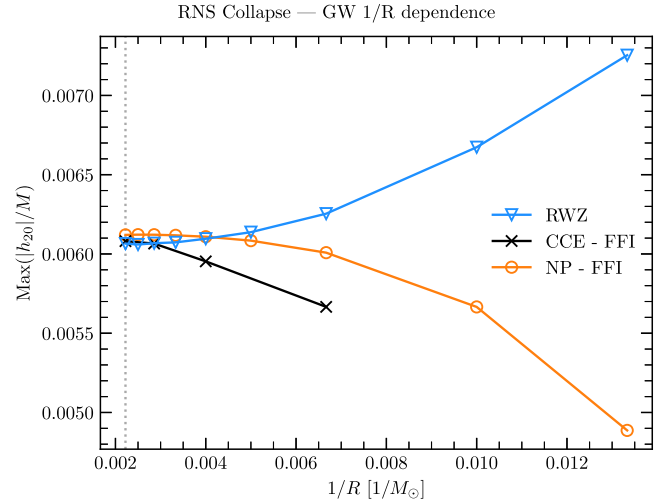


FIG. 12. Extraction radius dependence of the maximum strain amplitude of the $(2, 0)$ mode for the rotating collapse problem and different extraction algorithms. The dotted gray vertical line marks the radius with the best overall compatibility. Data refer to the highest-resolution simulation.

as a function of $1/R$: all the methods deliver a consistent waveform peak amplitude in the large- R limit. Despite its slow $1/R$ convergence and the noise, the RWZ extraction appears a robust choice for this problem, and it can help to identify systematics in the integration of ψ_4 waveforms. Further, we checked that an extrapolation of the RWZ waveform to null infinity significantly improves the waveform quality. The peak of the precursor around $u/M \sim 150$ lowers and become compatible to the CCE waveform computed with the world tube at $R = 450M_\odot$. Contrarily, the precursor of the CCE data computed with

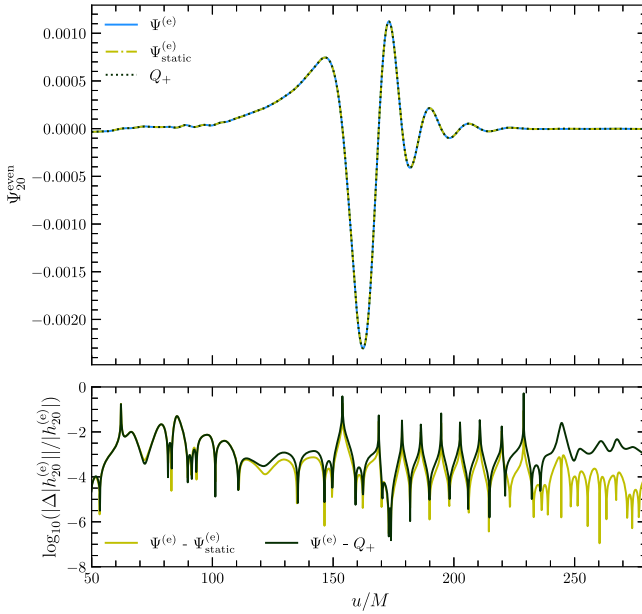
RNS Collapse — RWZ Master Functions comparison extracted at $R = 450M_\odot$ 

FIG. 13. RWZ (2, 0) mode for the rotating collapse problem extracted at $R = 450M_\odot$ and computed using different RWZ master functions. Top: even-parity master function extraction comparison $\Psi^{(e)}$ (solid blue), $\Psi^{(e)}_{\text{static}}$ (dot-dashed light green), and Q_+ (dotted dark green) normalized as per Eq. (21). Bottom: relative differences with respect to $\Psi^{(e)}$. Data refer to the highest-resolution simulation.

the world tube at $R = 150M_\odot$ remains unreliable. These results are shown in Appendix C.

Finally, we compare the different even-parity RWZ extraction master functions in Fig. 13. Despite having a dynamical background, relative differences are found of the order of 10^{-4} (away from a few zero crossing). They appear in line with what was found in the TOV problems (cf. Fig. 4). Therefore, we conclude that an extraction radius at $R \sim 450M_\odot$ is a robust choice for the metric extraction in this problem.

VII. BINARY BLACK HOLE SPACETIMES

To further test physical problems with nontrivial background and gauge dynamics, we consider an equal-mass, nonspinning, black hole binary in two different configurations: (i) a quasicircular configuration covering two orbits to merger, previously used as standard code benchmark [25,61], and (ii) a dynamical capture configuration considered in Ref. [31] with a close encounter followed then by a merger. Gravitational waves from these configurations are radiated in either the even-parity and odd-parity sector, but due to the $1 \leftrightarrow 2$ symmetry of the system, only the (2, 2), (2, 0), (3, 2), and (4, 4) modes are nonzero.

Binary black hole spacetimes are simulated on a domain $\Omega = [-1536M_\odot, 1536M_\odot]^3$ with $N_M = (128, 192)$ points

per direction. The domain is refined with $N_L = 10$ levels using the L_2 AMR strategy detailed by Rashti *et al.* [66]. The maximum resolution at the punctures is $h_{10} \simeq 0.0156M_\odot$. The CFL is set to 0.25, and the dissipation parameter is $\sigma = 0.2$. Spherical grids for the RWZ and NP extraction algorithms are located at $R = (80, 90, 100, 110, 120, 130, 140, 180, 220, 400)M_\odot$ while the world tubes for CCE are at $R = (100, 140, 220, 400)M_\odot$. Initial data are generated using the TwoPunctures code [76]. The initial data for the quasicircular configuration (that is such to yield only a couple of orbits up to merger) are generated with puncture ADM masses $M_1 = M_2 = M/2 = 0.505085M_\odot$ and ADM energy $E_{\text{ADM}}/M = 0.996$. For the dynamical capture, the puncture ADM masses are $M_1 = M_2 = M/2 = 0.5M_\odot$, ADM energy $E_{\text{ADM}}/M = 1.016$, and initial angular momentum $J_{\text{ADM}}/(\nu M^2) = 4.18$, where $\nu = M_1 M_2 / M^2 = 1/4$ is the symmetric mass ratio.

A. Quasicircular merger

Figure 14 shows the dominant (2, 2) strain mode (both real part and amplitude) from the three wave-extraction algorithms: (i) the RWZ metric procedure at $R_{\text{extr}} = 140M_\odot$ and (ii) ψ_4 at $R_{\text{extr}} = 140M_\odot$; the News $\mathcal{N}$ at $\mathcal{I}^+$. The methods prove consistent among themselves. Note that h_{22} was obtained from ψ_4 and the News $\mathcal{N}$ using FFI with a cutoff frequency $f_0 = 0.007/M$. The latter choice performs better than DTI due to the short duration of the signal, and it correctly captures most of the physical features. We further compare to the (longer) simulating extreme spacetimes (SXS):BBH:180 [77] waveform of the SXS catalog. The latter is extrapolated at infinity and aligned with the RWZ on the shaded time-domain window by suitably fixing an arbitrary relative time and phase shift.

The RWZ extracted function, $\Psi_{22}^{(e)}$, correctly captures the expected structure of the waveform, consistently with previous work that was using an extraction algorithm with fixed Schwarzschild-like coordinates (see, e.g., Ref. [78] and references therein). The amplitude agreement with CCE and NP (and with SXS:BBH:180) improves near the waveform peak, while some numerical artifact can be observed for RWZ and NP in the early part of the signal, before the junk. The amplitude of the RWZ waveform is smoother than the CCE and NP, especially at early times, $u/M \sim 50$. Around those times, both CCE and NP show an unphysical nonmonotonic behavior, which is mainly introduced by the FFI. The instantaneous gravitational wave frequency is also compatible among the different extraction algorithms. The most notable differences are present during the ringdown. NP and CCE data show larger oscillation at $u/M \gtrsim 200$, which are converging away with resolution. Early results with metric extraction (Q_+) also showed prominent oscillations [78], which are, however, significantly reduced at the resolution considered here. Phase differences among RWZ and NP multipoles at finite radius

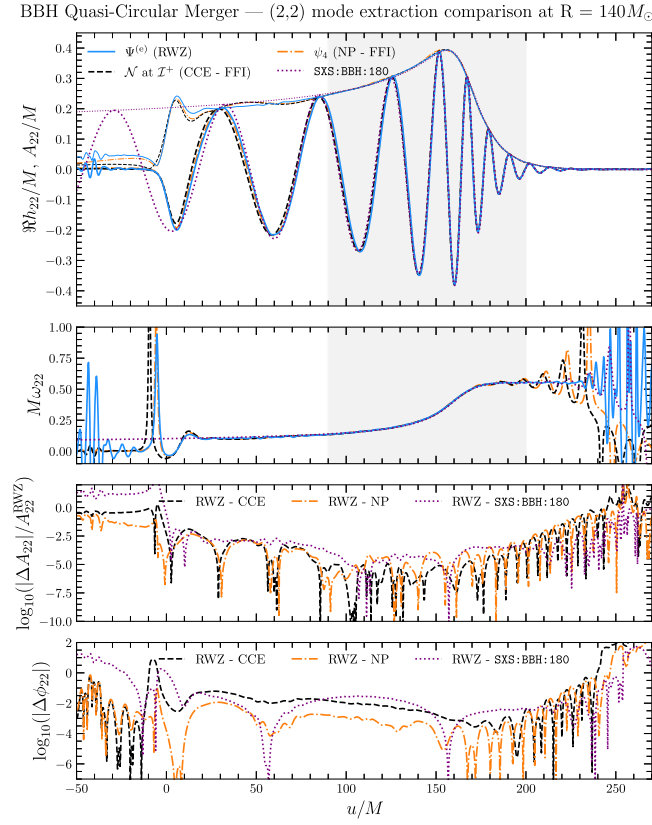


FIG. 14. Strain (2, 2) mode for the circular BBH merger at $R = 140M_\odot$. Different lines compare the results of the different extraction algorithms: RWZ (solid blue), CCE (dashed black), and NP (dot-dashed orange). Also shown is the SXS:BBH:180 waveform (dotted purple) aligned with the RWZ; the shaded area marks the alignment window. From top to bottom: amplitude and real part, frequency, amplitude differences, and phase differences with respect to the RWZ waveform. Data refer to the highest-resolution simulation.

($R = 140M_\odot$) are consistent with truncation errors and compatible with the SXS waveforms. Phase differences with respect to null infinity data can be a factor ~ 2 larger already for such a short waveform, which indicates larger extraction radii are required in order to obtain high-accuracy data. Both RWZ and NP extractions can be indeed improved by extrapolation; see Appendix C.

Finite extraction uncertainties are summarized in Fig. 15. The figure shows the peak amplitude for all extraction algorithms as a function of the extraction radius $1/R$. For comparison, we also show the value $A_{22}^{\text{SXS}}/M = 0.3919$ taken from SXS:BBH:180 extrapolated to infinite radius with $N = 3$. The best agreement between waveforms is obtained for $R = 140M_\odot$. At larger radii, the waveform's quality decreases because the extraction spheres are placed in refinement levels with progressively coarser resolutions. The amplitude becomes affected by significant uncertainties at extraction radii $R \gtrsim 180M_\odot$, which can decrease up

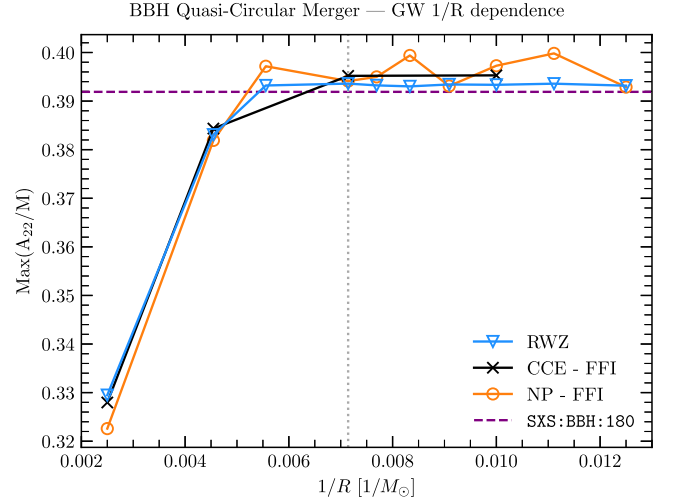


FIG. 15. Extraction radius dependence of the maximum strain amplitude (2, 2) for the quasicircular BBH merger and different extraction algorithms. The dotted gray vertical line marks the radius with the best overall compatibility. The dashed purple is the value from SXS:BBH:180, extrapolated to $\mathcal{I}^+$. Data refer to the highest-resolution simulation.

to 85% the amplitude for $R = 400M_\odot$ (with the chosen mesh resolution).

Higher modes (2, 0), (3, 2), and (4, 4) of the strain extracted at $R = 100M_\odot$ are shown in Fig. 16 for the different extraction algorithms. CCE and NP data are integrated with FFI using $f_0^{(\ell m)} = 2f_0/\max(1, m)$. This choice eliminates physical low-frequency features, in particular the nonlinear memory in the (2, 0) mode in CCE data, as can be observed in the top panel of the figure. Nonlinear memory can be captured in CCE data by using $f_0^{(20)} = 0.001/M$, but since we are not interested in studying this effect here, we keep for the CCE data the same integration as used for NP data. Overall, obtaining an accurate (2, 0) mode from such a short simulation appears rather challenging, and the different extraction algorithms deliver quantitatively different predictions. Concerning the other two modes, we find instead good agreement between the extraction algorithms. The figure shows some dephasing between CCE and finite radius data and that the (4, 4) mode NP data are more noisy than RWZ and CCE data (which can be improved by changing the frequency cutoff manually). Notably, for the (3, 2) mode, we show the RWZ waveform obtained from the master function $Q_\times$ (Schwarzschild coordinates) instead of from the $\Psi^{(0)}$. As discussed below, this appears the most robust choice for this particular mode.

We compare the different RWZ master functions for both even- and odd-parity sectors in Fig. 17. For the even parity, we show the (2, 2) mode, and for the odd parity, we show the (3, 2) mode. In the even-parity sector, we obtain similar

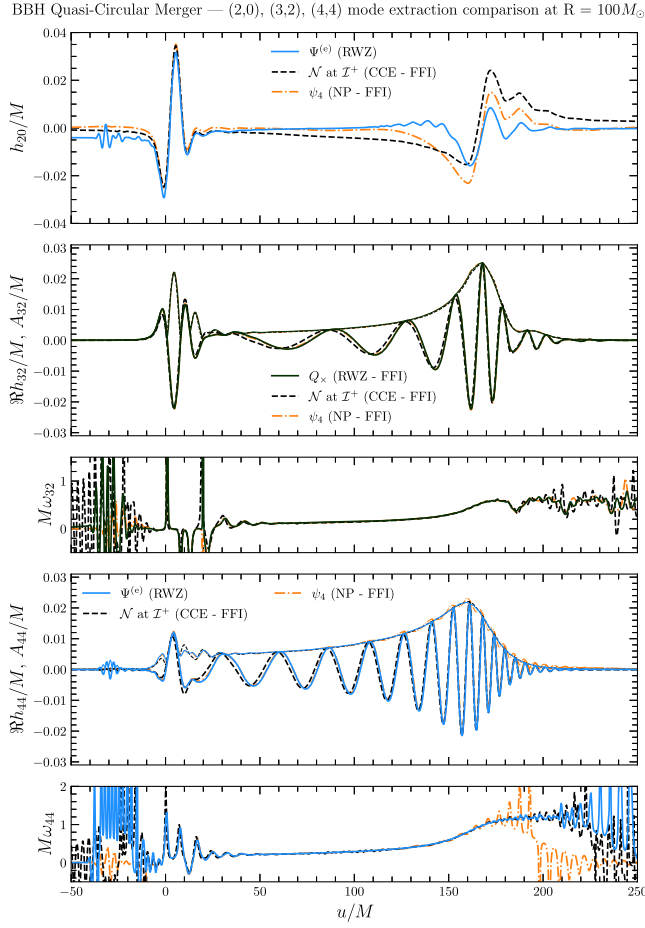


FIG. 16. Subdominant modes: (2, 0) (top), (3, 2) (middle, with frequency), and (4, 4) (bottom, with frequency) for the quasi-circular BBH merger extracted $R = 100M_\odot$. In each panel, different lines refer to different wave-extraction algorithms: RWZ (solid blue), CCE (dashed black), and NP (dotted-dashed orange). Data refer to the highest-resolution simulation.

results as discussed in previous problems. Amplitude relative differences with respect to $\Psi^{(e)}$ are of order $\sim 10^{-5}$ during the orbital phase and $\lesssim 10^{-3}$ at merger for both $\Psi_{\text{static}}^{(e)}$ and Q_+ . Phase differences are of order $\sim 10^{-3}$ rad at early times to grow up to $\sim 10^{-2}$ rad at merger; they remain compatible with truncation errors due to finite resolution.

More interesting is the odd-parity sector, where there are significant differences between the master functions in general coordinates $\Psi^{(o)}$ and the Schwarzschild coordinates master function $Q_\times$. The $\Psi^{(o)}$ amplitudes are larger and more noisy, with a significant amount of junk radiation at early times. More noise is also found in the instantaneous frequency evolution. Phase differences with respect to $Q_\times$ are also at the ~ 0.1 rad level, comparably larger than the dephasing in the even-parity mode discussed above. By inspecting the data, we identify the origin of these features as slowly convergent residual gauge effect due to the odd-parity $H_0^{(\ell m)}$ multipole [see Eqs. (25) and (41)]. The latter is

an integral of the shift vector which, in this example, is effectively worsening the performance of the covariant extraction when compared to $Q_\times$ (Schwarzschild coordinates.) This effect is present also in other higher modes and other binary problems, as we shall discuss below. Similarly to the RNS problem, the effects of the dynamical background are practically negligible for this BBH merger problem.

We have also compared waveforms for the different choices of the background's Schwarzschild radius prescriptions in this BBH problem. We obtain very similar results to the TOV problem. The areal and the average Schwarzschild radii deliver very comparable results with relative amplitude (phase) differences of order $\sim 10^{-6}$ ($\lesssim 10^{-5}$ rad). The $g\theta\theta$ and $g\phi\phi$ prescriptions also behave very similarly. The relative amplitude (phase) differences with respect to the average Schwarzschild radius are of order $\sim 10^{-3}$ ($\lesssim 10^{-2}$ rad). Any of these choices appear sufficiently robust for the considered setup and does not significantly impact the uncertainties discussed above.

B. Dynamical capture

The parameters detailed at the beginning of Sec. VII referring to case (ii) correspond to an initially unbound orbit which becomes bound due to the GW emission and lead to a merger after two encounters.

The capture dynamics is an interesting test for GW extraction algorithms because of the nontrivial morphology of the waveform. Figure 18 shows the dominant (2, 2) mode obtained with the different extraction algorithms at $R = 140M_\odot$. The amplitude and instantaneous frequency peak at each of the two encounters. The two peaks are separated by a low-frequency transient signal corresponding to the punctures reaching the apastron and returning on a bound orbit. The second peak corresponds to the merger, and it is followed by the ringdown signal of the remnant black hole. While the waveforms qualitatively agree in reproducing this morphology, significant differences are clearly present at the first peak and in the subsequent transient. The figure also shows for reference an EOB waveform obtained with TEOBResumS-Dalí [79,80] aligned in phase with the RWZ signal (alignment window marked with the shaded area). The initial data for the EOB evolution are chosen in order to minimize the mismatch against the RWZ waveform, following a procedure similar to the ones used in Ref. [81]. Such an EOB waveform is an important benchmark because it delivers a semianalytical prediction of the low-frequency transient between the encounters, which is captured by the Newtonian prefactor for generic motion [82]. Note that for the EOB waveform shown here we use a slightly different activation function for the next-to-quasicircular corrections adopted in the standard model to correct the EOB plunge waveform [79,80].

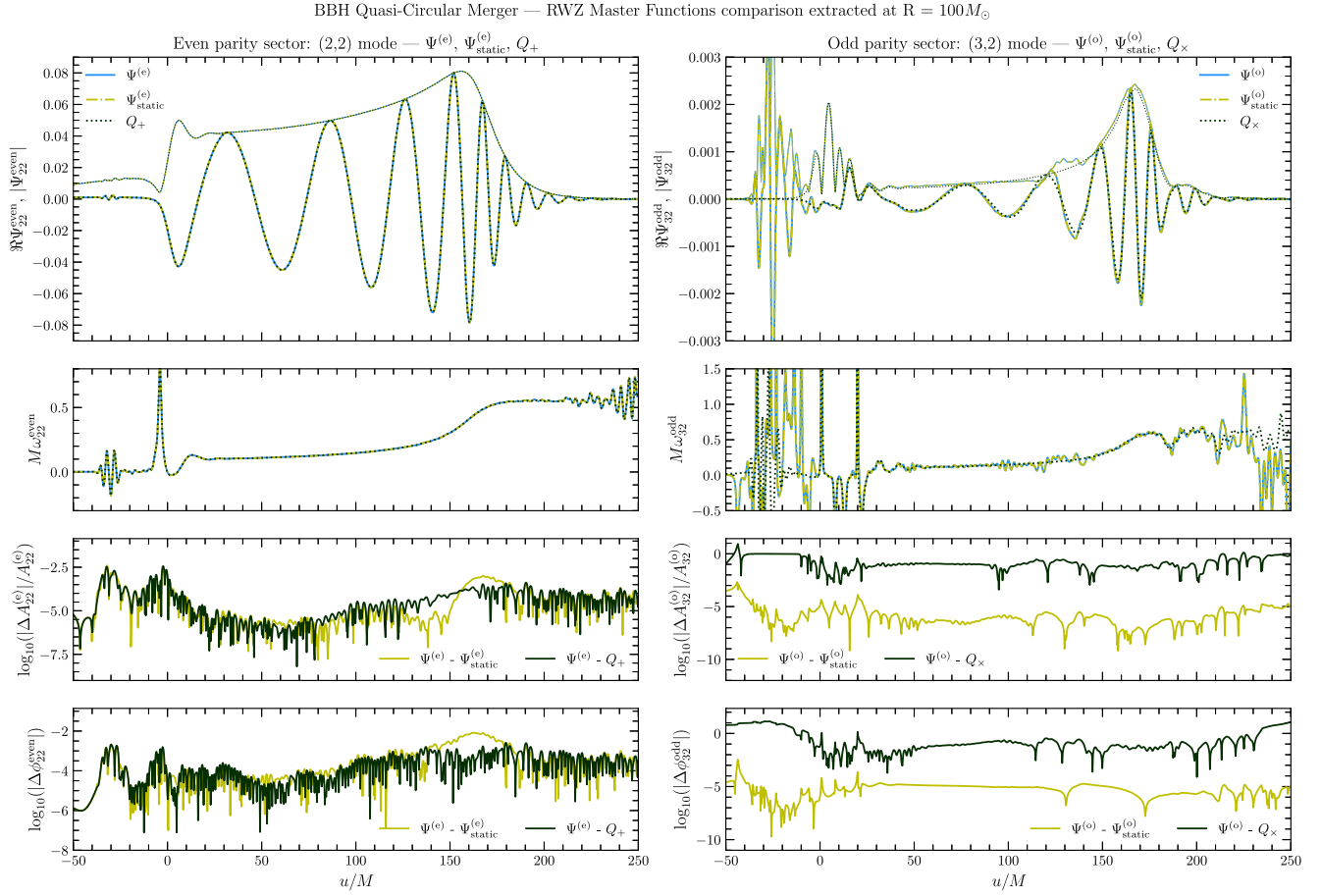


FIG. 17. RWZ even- and odd-parity modes for the BBH circular merger at $R = 100M_\odot$ and computed using different RWZ master functions. Left: even-parity (2, 2) master function extraction comparison $\Psi^{(e)}$ (solid blue), $\Psi_{\text{static}}^{(e)}$ (dot-dashed light green), and Q_+ (dotted dark green) normalized as per Eq. (21). Right: odd-parity (3, 2) master function extraction comparison $\Psi^{(o)}$ (solid blue), $\Psi_{\text{static}}^{(o)}$ (dot-dashed light green), and $Q_\times$ (dotted dark green) integrated and normalized as per Eq. (27). Panels in each columns show from top to bottom real part and amplitude, frequency, amplitude differences, and phase differences. Data refer to the highest-resolution simulation.

At the first encounter peak, both CCE and NP data show a double-peak structure which is unphysical. This artifact is induced by the integration of the ψ_4 converge away with increasing extraction radius (see also below). The data in the figure use FFI integration with a cutoff frequency $f_0 = 0.007/M$ [$f_0^{(\ell m)} = 2f_0/\max(1, m)$ for higher modes], similarly to what is done in Ref. [81]. The double peak artifact and the subsequent signal can be improved by lowering the frequency cutoff but that introduces noise and a drift in the ringdown part. In the absence of a physical cutoff frequency for the FFI, we also experimented with DTI but found less robust results than those shown in the figure.

During the low-frequency transient, the RWZ amplitude and frequency best match the EOB, while the CCE and NP data show qualitative differences. After merger, all the extraction algorithm become more compatible with similar features in the late ringdown as those discussed for the

BBH circular merger. Overall for this type of waveform, the RWZ extraction algorithm provides a robust alternative that can help to identify systematics in other algorithms.

The dependence of the waveforms on the extraction (or world-tube) radii is illustrated by Fig. 19, which shows the (2, 2) amplitude for various algorithms. The RWZ extraction shows a slower convergence with radius but eventually achieves the expected structure at $R \sim 140M_\odot$. By contrast, CCE and NP data retain the double-peak artifact discussed above. For larger radii $R \gtrsim 180M_\odot$, the amplitudes at the peaks starts to decrease considerably. This is again due to the resolution of the wave zone.

Regarding higher modes and the choice of different RWZ master functions, the dynamical capture simulation gives analogous results to the circular merger. Figure 20 shows the RWZ (4, 4) and (3, 2) modes computed from $\Psi^{(e/o)}$, $\Psi_{\text{static}}^{(e/o)}$ and $Q_{+/\times}$. Very consistent results are found in the even sector for any choice of the master function. Note

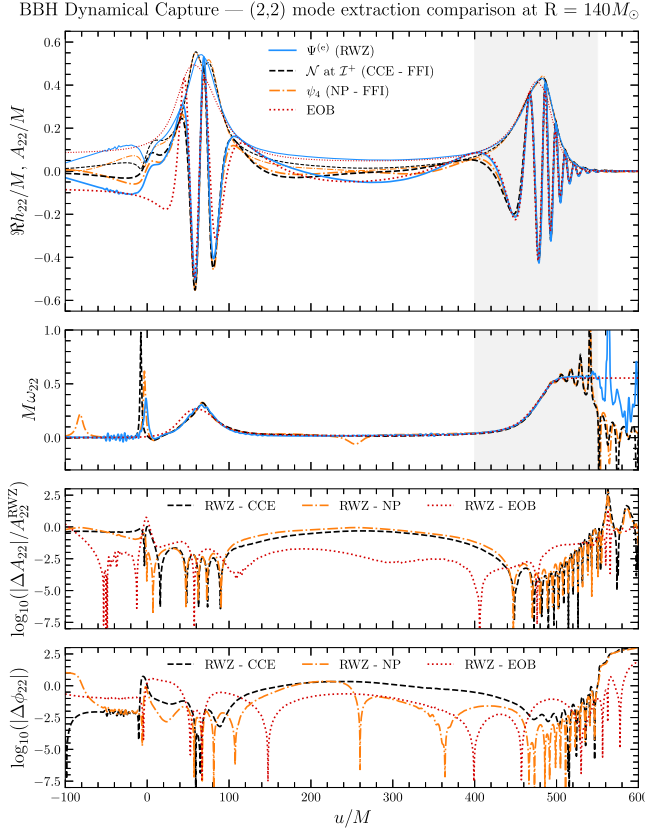


FIG. 18. Strain (2, 2) mode for a BBH dynamical capture at $R = 140M_\odot$. Different lines compare the results of the different extraction algorithms: RWZ (solid blue), CCE (dashed black), and NP (dot-dashed orange). Also shown is a EOB prediction (dotted red) aligned with the RWZ; the shaded area marks the alignment window. From top to bottom: amplitude and real part, frequency, amplitude differences, and phase differences with respect to the RWZ waveform. Data refer to the highest-resolution simulation.

that there are only subtle differences at the peaks with respect to $\Psi_{\text{static}}^{(e)}$ in the (4, 4) mode, which are mildly reduced at lower distance. By contrast, the odd-parity waveform extraction with $\Psi^{(o)}$ and $\Psi_{\text{static}}^{(o)}$ are more noisy than the $Q_\times$. Unsurprisingly, due to the same gauge employed in this simulation and in the circular merger, the latter choice appears more robust for the odd modes.

VIII. BINARY NEUTRON STAR SPACETIME

For a final problem, we consider a ten-orbits binary neutron star merger simulation previously simulated in Refs. [83–85]. To our knowledge, metric waveform extraction in such long BNS simulations have never been previously considered. The stars have isolation masses

$M_1 = M_2 = M/2 = 1.35M_\odot$ and are described by the SLy EOS and irrotational fluid. They are initially separated by a coordinate distance $d = 52.42$ km. Initial data are generated using the LORENE library [86].

The simulations use a domain $\Omega = [-1024M_\odot, 1024M_\odot]^3$ with $N_M = 160$ and $N_L = 6$ refinement levels ($h_6 = 0.2M_\odot$) with AMR strategy as detailed by Daszuta *et al.* [63]. The CFL is set to 0.25, and the dissipation parameter is $\sigma = 0.5$. The extraction spheres the RWZ and NP algorithms are located at $R = 100, 200, 300, 400, 500, 600, 700, 800, 900M_\odot$, while the world tubes for the CCE are at $R = 200, 400, 600, 800M_\odot$.

The dominant (2, 2) mode of the GW strain is shown in Fig. 21 for the three extraction algorithms. Waveforms are also compared to a EOB waveform generated with TEOBResumS-Dalí. The RWZ extraction ($\Psi_{22}^{(e)}$) correctly captures the well-known *inspiral-merger-postmerger* structure of the waveforms, and it is entirely compatible with other extraction algorithms. Relative amplitude differences $\lesssim 10^{-5}$, which is well below the uncertainty due to truncation errors. Similarly, phase differences at finite extraction radii are of order $\lesssim 10^{-2}$ rad and compatible with the EOB accuracy. CCE data at $\mathcal{I}^+$ highlight some significant dephasing with finite extraction data, thus suggesting the need of extrapolation in order to obtain precise data for, e.g., EOB modeling [87]. Similarly to other problems, a simple extrapolation of the RWZ multipole significantly improves the agreement with CCE data; see Appendix C.

Finite-radius extraction effects in the waveform’s amplitude are summarized in Fig. 22. The RWZ and the NP amplitudes become consistent at radii $R > 200M_\odot$. Comparing to BBH simulations, finite-radius effects in the RWZ are less severe since in this problem it is possible to reliably extract waveforms at larger radii. Nonetheless, RWZ data at $R = 900M_\odot$ start to show unphysical oscillations due to insufficient resolution in the wave zone.

Finally, we compare the different choices for the RWZ master functions. For the (2, 2) mode, we find that $\Psi_{22}^{(e)}$, $\Psi_{\text{static } 22}^{(e)}$, and Q_{+22} are essentially equivalent at the optimal radius $R = 800M_\odot$. Relative amplitude (phase) differences are of order $\lesssim 10^{-6}$ (10^{-5} rad). Figure 23 shows the (4, 2) and (3, 2) modes computed with the difference master function choices at $R = 200M_\odot$. Results are in line with those discussed above for BBH, but here the amplitude (relative) and phase differences among the master functions are an order of magnitude smaller. Moreover, we stress again that with the Γ -driver shift odd-parity modes are more robustly obtained from the $Q_\times$ (Schwarzschild coordinates) than from $\Psi^{(o)}$.

BBH Dynamical Capture — GW amplitude radial dependence

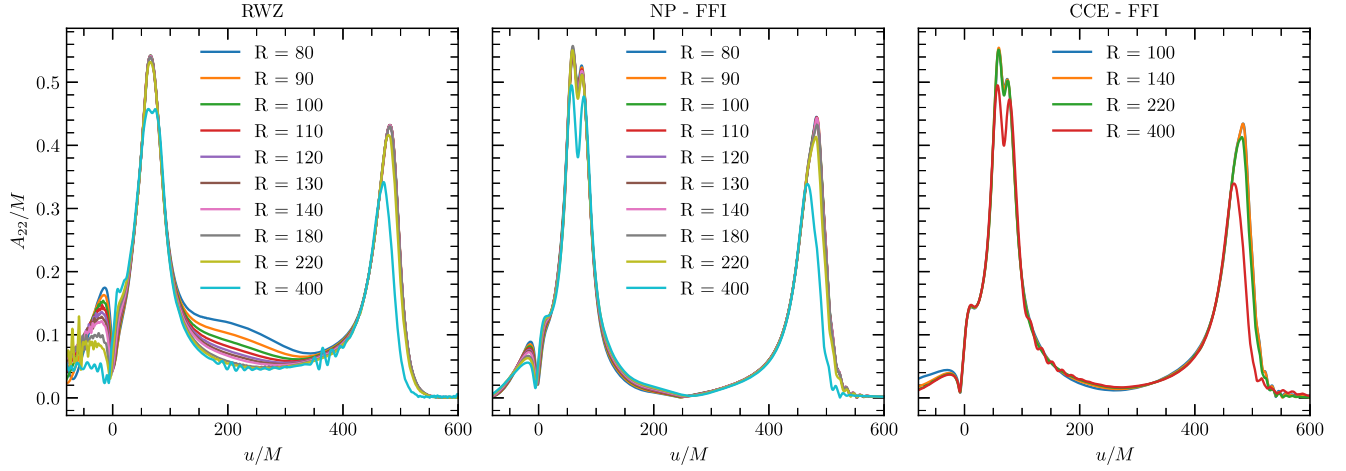


FIG. 19. Extraction radius dependence of the strain (2, 2) mode for the BBH dynamical capture. Panels from left to right: RWZ, NP, and CCE extraction. For each panel, different lines show different extraction radii (in units of $M_\odot$). Data refer to the highest-resolution simulation.

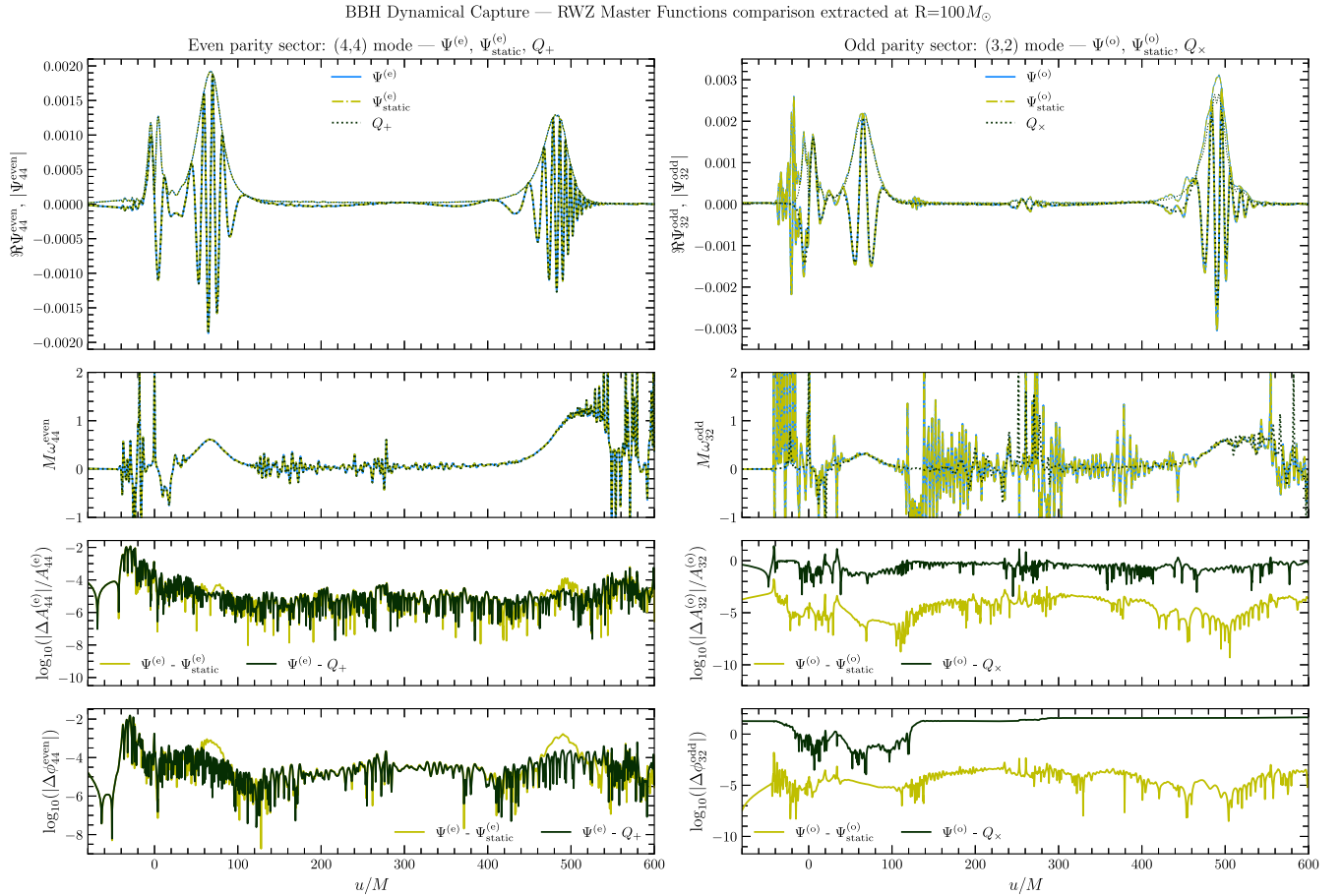


FIG. 20. RWZ even- and odd-parity modes for the BBH dynamical encounter at $R = 100M_\odot$ and computed using different RWZ master functions. Left: even-parity (4, 4) master function extraction comparison $\Psi^{(e)}$ (solid blue), $\Psi_{\text{static}}^{(e)}$ (dot-dashed light green), and Q_+ (dotted dark green) normalized as per Eq. (21). Right: odd-parity (3, 2) master function extraction comparison $\Psi^{(o)}$ (solid blue), $\Psi_{\text{static}}^{(o)}$ (dot-dashed light green), and $Q_\times$ (dotted dark green) integrated and normalized as per Eq. (27). Panels in each columns show from top to bottom: real part and amplitude, frequency, amplitude differences, and phase differences. Data refer to the highest-resolution simulation.

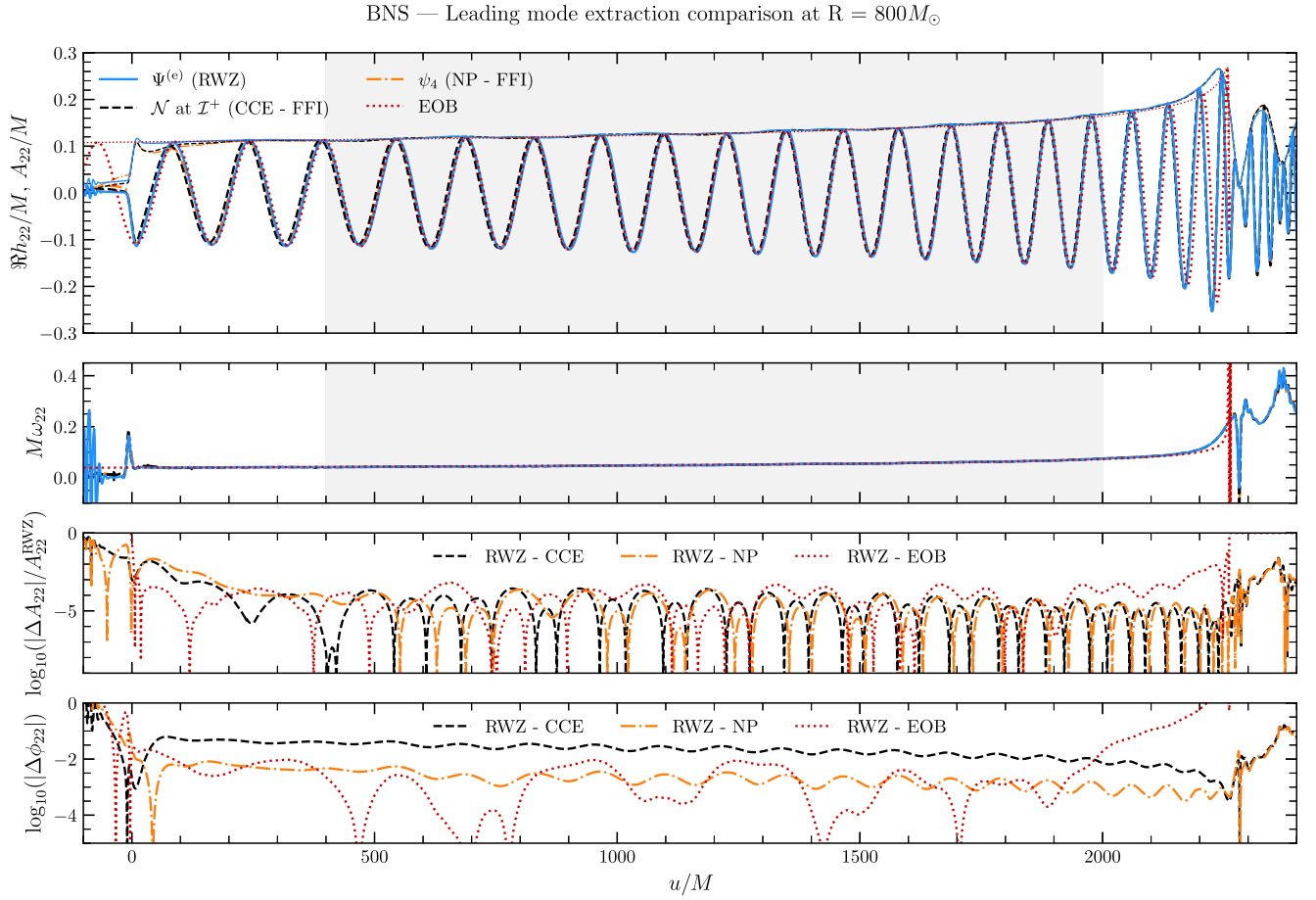


FIG. 21. Strain (2, 2) mode for the circular BNS merger at $R = 800M_\odot$. Different lines compare the results of the different extraction algorithms: RWZ (solid blue), CCE (dashed black), and NP (dot-dashed orange). Also shown is a longer EOB waveform (dotted red) aligned with the RWZ; the shaded area marks the alignment window. From top to bottom: amplitude and real part, frequency, amplitude differences, and phase differences with respect to the RWZ waveform.

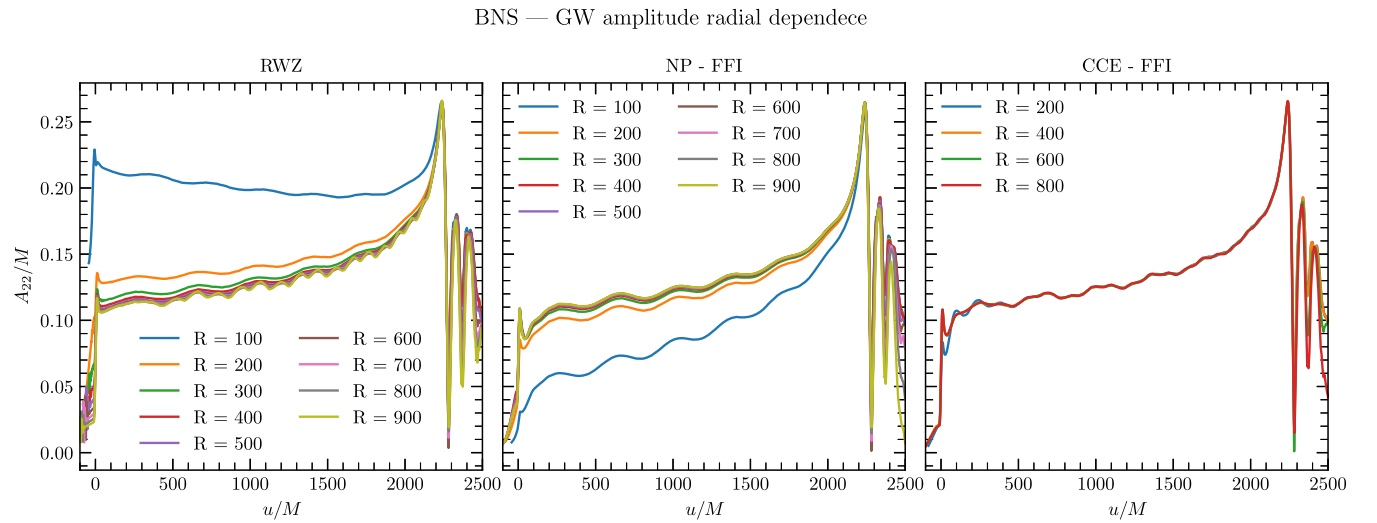


FIG. 22. Extraction radius dependence of the strain (2, 2) mode for the circular BNS merger. Panels from left to right: RWZ, NP, and CCE extraction. For each panel, different lines show different extraction radii (in units of $M_\odot$).

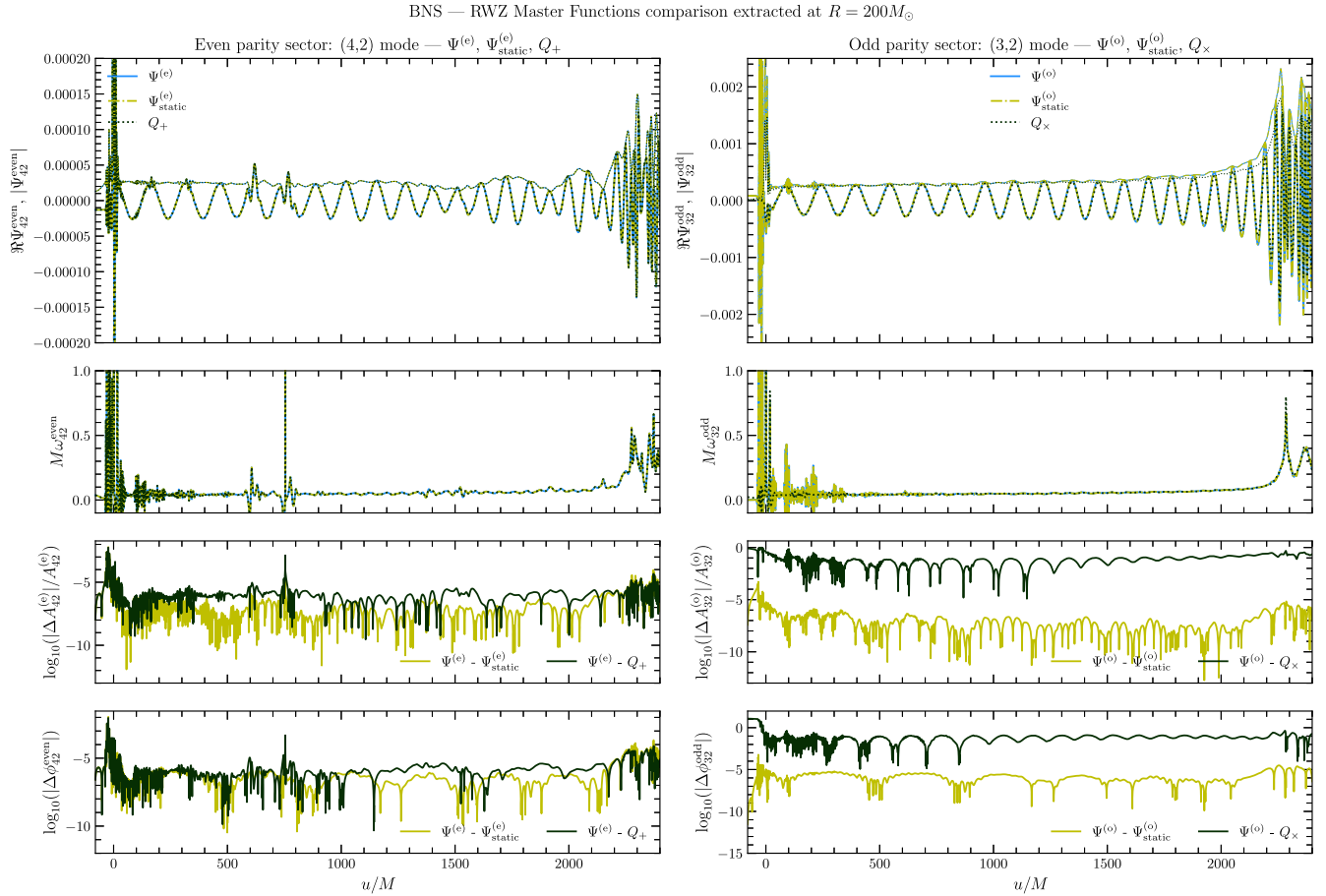


FIG. 23. RWZ even- and odd-parity modes for the BNS circular merger at $R = 800M_\odot$ and computed using different RWZ master functions. Left: even-parity (4, 2) master function extraction comparison $\Psi^{(e)}$ (solid blue), $\Psi_{\text{static}}^{(e)}$ (dot-dashed light green), and Q_+ (dotted dark green) normalized as per Eq. (21). Right: odd-parity (3, 2) master function extraction comparison $\Psi^{(o)}$ (solid blue), $\Psi_{\text{static}}^{(o)}$ (dot-dashed light green), and Q_x (dotted dark green) integrated and normalized as per Eq. (27). Panels in each columns show from top to bottom: real part and amplitude, frequency, amplitude differences, and phase differences.

IX. CONCLUSION

In this paper, we have revisited the problem of gravitational-waves extraction in numerical relativity using the covariant and gauge-invariant formalism of spherical spacetime perturbations.

The first part of the paper summarizes the formalism introduced by Moncrief [4,5] and Gerlach and Sengupta [6] and further developed by other authors [7–10]. Ready-to-use expressions for the most general covariant and gauge-invariant even- and odd-parity master functions are reported for the first time in terms of the $(3+1)$ -metric multipoles. The presentation also connects the different conventions and notations employed in the literature; the hope is to provide the reader a consistent and complete summary of results that appeared over several decades. Technical aspects of our new implementation of the extraction algorithm in the $(3+1)$ numerical relativity code GR-Athena++ are also detailed.

The central results are given by Eqs. (20) and (25), which are the even- and odd-parity master functions for the most general choice of the spherical background. These functions directly provide the multipoles of the strain, Eq. (1). They reduce to Eqs. (19) and (26) in case of a static background and to Moncrief [4,5] variables via Eqs. (21) and (27) for a background in Schwarzschild coordinates.

The second part of the paper discusses a systematic assessment of the metric extraction algorithm based on a comprehensive suite of $(3+1)$ simulations. The benchmark problems are perturbed TOV stars, gravitational collapse of a rapidly rotating neutron star, a BBH circular merger and a dynamical capture, and a ten-orbit BNS circular merger. For most of these 3D simulations, it is the first time that a covariant and gauge-invariant metric extraction algorithm is considered and compared to curvature and CCE waveforms. Also, to the best of our knowledge, it is the first time that TOV w -modes are explored in 3D complete simulations without symmetries; cf. Ref. [72].

Our numerical experiments demonstrate common features of the metric extraction algorithm across the different benchmarks.

First, we find that metric extraction is robust in all the considered scenarios. Metric waveforms extracted are of comparable quality to curvature waveforms extracted at the same finite radius. Metric extraction is particularly valuable in identifying waveform systematics for problems in which the reconstruction of the strain from the ψ_4 multipoles is ambiguous. Notable examples are the rotational collapse and the dynamical capture. The main drawback observed in the metric extraction when compared to curvature extraction is a slower convergence with the extraction and a slightly higher numerical noise. The latter is more evident in the computation of higher modes.

Second, we provide a direct comparison of the different choices for the gauge-invariant master functions. In the even-parity sector, any choice of the master function is robust for all the problems. Differences in both phase and amplitude of the RWZ multipoles are significantly below the uncertainties introduced by the choice of extraction radius (and resolution) and generically smaller than differences with other extraction algorithms. In the odd-parity sector, we instead find that the gauge choice in our simulations, in particular the Γ -driver shift, introduces some significant systematic effect for simulations that require a nontrivial shift (notably compact binaries.) As a consequence, assuming Schwarzschild coordinates for the background, i.e., considering the $Q_\times$ multipoles, can be a better choice for such simulations. This is an unexpected result, but it can be understood by noting that the gauge-dependent odd multipole $H_0^{(\ell m)}$ (a projection of the shift components) enters directly Eqs. (25) and (26), but not Eq. (22). We note this is not in contradiction with the findings of Pazos *et al.* [13], since that work considers perturbations of a stationary spacetime and employed harmonic coordinates. Further, the different choices of the Schwarzschild radius are all found robust as they introduce uncertainties typically smaller than the choice of finite extraction radius. The average Schwarzschild radius can be used as default due to its general character.

Third, we provide a direct comparison to CCE waveforms which are propagated to null infinity from finite radius world tubes. Compared to “optimal” extraction spheres, null infinity waveforms show some significant phase differences, in particular for compact binary simulations. Such differences can become a dominant source of uncertainty if higher mesh resolutions than those considered in our benchmarks are employed. However, CCE waveforms also have uncertainties associated to the choice of the world tube [40–42]. We find that a simple extrapolation to null infinity can deliver rather precise metric waveforms compatible in phase to CCE. These extrapolated waveforms are particularly accurate for problems that allow extraction at sufficiently large radii as, for example,

the considered BNS merger simulation. A companion paper explores yet another technique to propagate (metric) waveforms to null infinity using perturbative simulations with hyperboloidal foliation [58]. That technique is naturally associated to spherical spacetime perturbations, and it employs the RWZ data extracted at a coordinate sphere as boundary data to propagate to null infinity.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

APPENDIX A: NOTATION AND CONVENTIONS

We use geometric units $c = G = 1$ and signature $(-, +, +, +)$; partial derivatives are indicated as ∂ . A 4-metric is indicated explicitly as ${}^{(4)}g_{\mu\nu}$ with indices $\mu, \nu = 0, \dots, 3$. We employ the standard notation for the 3-metric γ_{ij} with indices $i, j = 1, 2, 3$; the shift vector β^i ; and the lapse function α . The line element is

$$ds^2 = -(\alpha^2 - \beta_i \beta^i) dt^2 + 2\beta_i dt dx^i + \gamma_{ij} dx^i dx^j. \quad (\text{A1})$$

1. Schwarzschild background

Schwarzschild spacetime is given by the direct product of a two-dimensional Lorentzian manifold L^2 and the 2-spheres, i.e., $\mathcal{M} = L^2 \times S^2$. This background spacetime

is spherically symmetric, but the coordinates on L^2 are not specified. The metric on S^2 is written as σ_{ab} with indices $a, b = 2, 3$. The covariant derivative is indicated as ∇_a . The volume form is indicated as ϵ_{cd} ($\epsilon_{cd}\epsilon^{ce} = \sigma_d^e$). On S^2 , we use standard latitude-longitude coordinates (θ, ϕ) , and thus $\sigma_{ab} = \text{diag}(1, \sin^2 \theta)$ and the nonzero components of the Levi-Civita tensor are $\epsilon_{\theta\phi} = \sin \theta = -\epsilon_{\phi\theta}$. The background 2-metric on L^2 is written as g_{AB} with indices $A, B = 0, 1$. The covariant derivative on L^2 is indicated as ∇_A . The (antisymmetric) volume form is $\epsilon_{AB} = \sqrt{\det|g_{CD}|}\tilde{\epsilon}_{AB}$, where $\tilde{\epsilon}_{AB}$ is the totally antisymmetric symbol and $\epsilon^{AB} = (-\tilde{\epsilon}_{AB})/\sqrt{\det|g_{CD}|}$. The generic coordinates on L^2 are written as x^A where x^0 is a time and x^1 is a radial coordinate that does not need to be the areal radius.

The background 4-metric is written as

$${}^{(4)}g_{\mu\nu} = \begin{pmatrix} g_{AB} & 0 \\ 0 & r^2 \sigma_{ab} \end{pmatrix}, \quad (\text{A2})$$

where r is the areal radius defined from the S^2 volume,

$$4\pi r^2 = \int_{S^2} \sqrt{\det(\sigma_{ab})} = \int_0^{2\pi} \int_0^\pi \sin \theta d\theta d\phi. \quad (\text{A3})$$

The background spacetime for the wave-extraction algorithm is characterized by the mass M of the spacetime that can be defined in coordinate-invariant way. Following Sarbach and Tiglio [9] and Martel and Poisson [10], we introduce the 1-form

$$dr = \partial_A r dx^A = r_A dx^A, \quad (\text{A4})$$

where $r_A \equiv \partial_A r$. The coordinate-invariant definition of the mass of the system is

$$M = \frac{r}{2}(1 - N), \quad (\text{A5})$$

where $N := r_A r^A$ with $r^A = g^{AB} r_B$. Note that our N corresponds to Martel and Poisson [10] function f . Assuming, for example, Schwarzschild coordinates $x^A = (t, r)$, where r is the areal radius of the sphere, one obtains $r_A = (0, 1)$ and $t^A = (1, 0)$. The inverse metric g^{AB} can be written in the frame defined by (t^A, r^A) as

$$g^{AB} = N^{-1}(-t^A t^B + r^A r^B). \quad (\text{A6})$$

As a result, the vector r^A explicitly reads

$$r^A = \begin{pmatrix} g^{01} \\ g^{11} \end{pmatrix}, \quad (\text{A7})$$

and the invariant mass is

$$M = \frac{r}{2}(1 - g^{11}). \quad (\text{A8})$$

This equation identifies in a coordinate-invariant way the component g^{11} of the metric,

$$g^{11} = 1 - \frac{2M}{r}. \quad (\text{A9})$$

This is not the case for the other components of the metric with upper indices that, in general, will depend on the chosen time coordinate. The metric components with lower indices can depend on time, too, in general coordinates x^A . However, requiring that the metric satisfies Einstein equations in vacuum still implies that M is time independent [9].

2. Spherical harmonics

Scalar spherical harmonics are indicated as $Y_{\ell m}(\theta, \phi)$ and are defined by

$$\sigma^{ab} \nabla_a \nabla_b Y_{\ell m} = -\lambda Y_{\ell m}, \quad (\text{A10})$$

where $\lambda = \lambda(\ell) := \ell(\ell + 1)$. They are normalized such that

$$\int Y_{\ell m} Y_{\ell' m'}^* d\Omega = \delta_{\ell m \ell' m'}, \quad (\text{A11})$$

where $d\Omega = \sin \theta d\theta d\phi$, and so that $Y_{00} = 1/\sqrt{4\pi}$.

Tensor fields on S^2 can be decomposed in a basis with definite parity. A 1-form on S^2 can be decomposed in vector spherical harmonics,

$$V_a = \sum_{\ell=1}^{\infty} \sum_{m=-\ell}^{\ell} \left(v_{\text{even}}^{(\ell m)} Y_a^{(\ell m)} + v_{\text{odd}}^{(\ell m)} S_a^{(\ell m)} \right), \quad (\text{A12})$$

where $v_{\text{even/odd}}^{(\ell m)}$ are the multipoles and the vector spherical harmonics

$$Y_a^{(\ell m)} := \nabla_a Y_{\ell m} \quad (\text{A13a})$$

$$S_a^{(\ell m)} := \epsilon_{cd} \nabla_a Y_{\ell m} = \epsilon_{ab} \sigma^{bc} \nabla_c Y_{\ell m} \quad (\text{A13b})$$

have even and odd parity, respectively. The basis elements obey the orthogonality relations

$$\int \sigma^{ab} Y_a^{(\ell m)} Y_b^{(\ell' m')*} d\Omega = \lambda \delta_{\ell \ell'} \delta_{mm'} \quad (\text{A14a})$$

$$\int \sigma^{ab} S_a^{(\ell m)} S_b^{(\ell' m')*} d\Omega = \lambda \delta_{\ell \ell'} \delta_{mm'} \quad (\text{A14b})$$

$$\int \sigma^{ab} Y_a^{(\ell m)} S_b^{(\ell' m')*} d\Omega = 0. \quad (\text{A14c})$$

Using the (θ, ϕ) coordinates on S^2 , the above components explicitly read

$$Y_a^{(\ell m)} = (Y_\theta^{(\ell m)}, Y_\phi^{(\ell m)}) = (\partial_\theta Y_{\ell m}, \partial_\phi Y_{\ell m}) \quad (\text{A15a})$$

$$S_a^{(\ell m)} = (S_\theta^{(\ell m)}, S_\phi^{(\ell m)}) = \left(-\frac{1}{\sin \theta} \partial_\phi Y_{\ell m}, \sin \theta \partial_\theta Y_{\ell m} \right). \quad (\text{A15b})$$

Consequently, the multipoles of a 1-form can be computed as

$$v_{\text{even}}^{(\ell m)}(\ell m) = \frac{1}{\lambda} \int \left(V_\theta \partial_\theta Y_{\ell m}^* + \frac{1}{\sin^2 \theta} V_\phi \partial_\phi Y_{\ell m}^* \right) d\Omega \quad (\text{A16a})$$

$$v_{\text{odd}}^{(\ell m)}(\ell m) = \frac{1}{\lambda} \int \frac{1}{\sin \theta} (-V_\theta \partial_\phi Y_{\ell m}^* + V_\phi \partial_\theta Y_{\ell m}^*) d\Omega. \quad (\text{A16b})$$

A 2-tensor T_{ab} on S^2 can be decomposed in tensor spherical harmonics as

$$T_{ab} = \sum_{\ell=2}^{\infty} \sum_{m=-\ell}^{\ell} \left(K^{(\ell m)} \sigma_{ab} Y_{\ell m} + G^{(\ell m)} Y_{ab}^{\ell m} + H^{(\ell m)} S_{ab}^{(\ell m)} \right), \quad (\text{A17})$$

where the multipoles $K^{(\ell m)}$ and $G^{(\ell m)}$ have even parity and $H^{(\ell m)}$ has odd parity. These tensor multipoles are computed by similar projections as those of vector multipoles. The tensor spherical harmonics basis of even and odd parity are, respectively [89,90],

$$Y_{\ell m} \quad \text{and} \quad Y_{ab}^{(\ell m)} := \nabla_a \nabla_b Y_{\ell m} + \frac{\lambda}{2} \sigma_{ab} Y_{\ell m}, \quad (\text{A18a})$$

$$S_{ab}^{(\ell m)} := \nabla_{(a} S_{b)}^{(\ell m)} = \frac{1}{2} \left(\nabla_a S_b^{(\ell m)} + \nabla_b S_a^{(\ell m)} \right). \quad (\text{A18b})$$

Explicit expression in (θ, ϕ) coordinates can be found in, e.g., Appendix A of the work by Martel and Poisson [10]. The basis elements obey the orthogonality relations

$$\int \sigma^{ab} \sigma^{cd} Y_{ab}^{(\ell m)} Y_{cd}^{(\ell' m')*} d\Omega = \frac{1}{2} \lambda (\lambda - 2) \delta_{\ell \ell'} \delta_{mm'} \quad (\text{A19a})$$

$$\int \sigma^{ab} \sigma^{cd} S_{ab}^{(\ell m)} S_{cd}^{(\ell' m')*} d\Omega = \frac{1}{2} \lambda (\lambda - 2) \delta_{\ell \ell'} \delta_{mm'} \quad (\text{A19b})$$

$$\int \sigma^{ab} \sigma^{cd} Y_{ab}^{(\ell m)} S_{cd}^{(\ell' m')*} d\Omega = 0. \quad (\text{A19c})$$

The $Y_{ab}^{(\ell m)}$ basis introduced by Mathews [89] and Zerilli [90] is sometimes also indicated as $Z_{ab}^{(\ell m)}$. The tensor spherical harmonics $Y_{ab}^{(lm)}$ and $S_{ab}^{(lm)}$ can be related to spin-weighted spherical harmonics with spin $s = -2$ [91] and to the pure spin tensor harmonics $T_{AB}^{\text{E2}(\ell m)}, T_{AB}^{\text{B2}(\ell m)}$ of Thorne [92]; see Appendix A of Martel and Poisson [10]. Note that Regge and Wheeler [2] used an alternative even-parity tensor basis defined without the trace term in Eq. (A18a), i.e., $Y_{ab\text{RW}}^{(\ell m)} := \nabla_a \nabla_b Y_{\ell m}$. With this choice, however, the tensor harmonics are not linearly independent.

APPENDIX B: DETAILS ON NUMERICAL IMPLEMENTATION

1. Integrals on the sphere

Integrals of functions $f(\theta, \phi)$ on the 2-spheres are computed using Gauss-Legendre quadratures,

$$I_{S^2}[f] := \int f(\theta, \phi) d\Omega \approx \sum_{ij} w_{ij} f(\theta_i, \phi_j). \quad (\text{B1})$$

The grid in the longitude coordinate $\phi \in (0, 2\pi)$ has nodes

$$\phi_j = \frac{2\pi}{N_\phi} \left(j + \frac{1}{2} \right), \quad j = 0, \dots, N_\phi - 1, \quad (\text{B2})$$

while the grid in the latitude coordinate $\theta \in (0, \pi)$ has nodes θ_i from the Gauss-Legendre nodes x_i ,

$$\theta_i = \arccos(x_i), \quad i = 0, \dots, N_\theta - 1. \quad (\text{B3})$$

The integral weights are computed as

$$w_{ij} = \frac{2\pi}{N_\phi} w_i, \quad (\text{B4})$$

where w_i are the Gauss-Legendre quadrature weights. Polynomials in x of degree $2N_\theta - 1$ are integrated exactly by the scheme.

Numerical experiments with TOV spacetimes indicate that the background computation requires at least $N_\theta = N_\phi/2 = 32$ to obtain the Schwarzschild radius to 1% precision. Nevertheless, Gauss-Legendre quadratures achieve better precision with $N_\theta = N_\phi/2 = 128$ especially for more complex problems such as binaries and higher modes.

2. Metric and derivatives

The $(3+1)$ -metric and its spatial derivatives are computed on the Cartesian grid and then interpolated on a sphere with given isotropic radius R . First derivatives are calculated with centered finite differencing stencils of the same order used in the evolution algorithm ($n = 4, 6$) and

interpolated with Lagrangian polynomials of order $2n - 1$. Second spatial derivatives are consistently obtained from the interpolating polynomials. The metric's first time derivatives are computed from the definition of the extrinsic curvature and then interpolated. The metric's mixed time-space derivatives are obtained from the interpolating polynomial. For simplicity, we instead do not implement terms proportional to second time derivatives. The choice is justified *a posteriori* by the comparison Ψ_{static} and of Ψ that, already without these subdominant contributions, show very small differences in all our simulations.

APPENDIX C: R-EXTRAPOLATED RWZ MASTER FUNCTIONS

As mentioned in the above text, the quality of RWZ waveforms can be improved by a simple extrapolation in $1/R$ and retarded time. Our extrapolation procedure follows Eq. (4) of Nakano *et al.* [35] with a modification analogous to their Eq. (29),

$$\Psi_{\ell m}^{(e,o)}(u) \Big|_{r=\infty} = \left(1 - \frac{2M}{r}\right) \left(\Psi_{\ell m}^{(e,o)}(u, r) - \frac{\ell(\ell+1)}{2r} \int_0^u dt \Psi_{\ell m}^{(e,o)}(t, r) \right). \quad (\text{C1})$$

We show here selected results for two representative problems: the BNS merger and the rotational collapse.

Extrapolated waveforms for the BNS are shown in Fig. 24. We obtain phase differences with respect to the

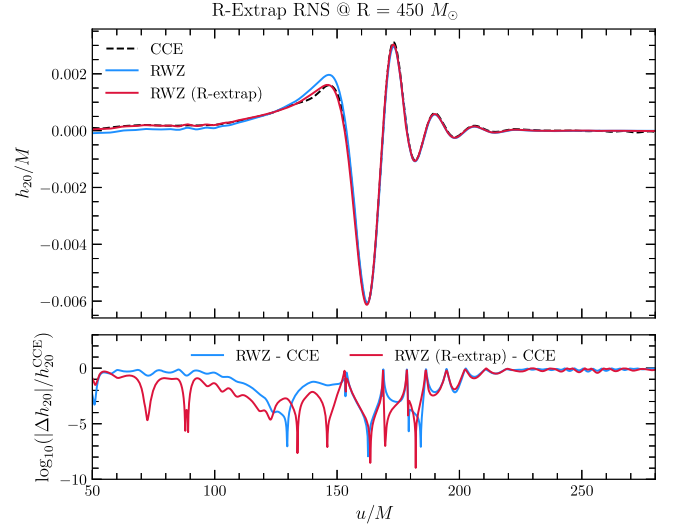


FIG. 25. Strain $(2, 0)$ mode for the RNS collapse at $R = 450 M_\odot$. Different lines compare the results of the different extraction algorithms: RWZ (solid blue), RWZ R-extrapolated (solid red), and CCE (dashed black). Top: amplitude and real parts. Bottom: amplitude relative differences with respect to the CCE waveform.

CCE ~ 2 orders of magnitude smaller than those obtained with finite radius extraction. With this extrapolation waveform extraction, uncertainties become negligible with respect to mesh resolution uncertainties.

Figure 25 shows extrapolated waveforms for the collapse. Here, the main difference with respect to CCE is in

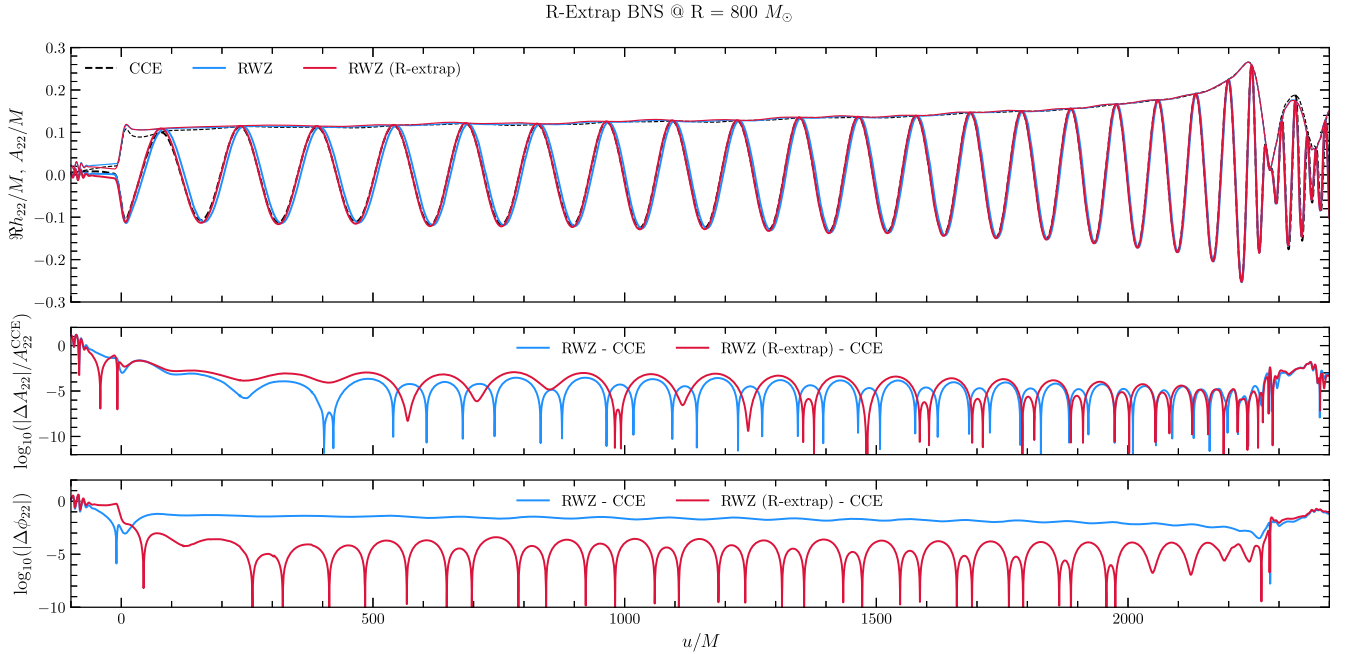


FIG. 24. Strain $(2, 2)$ mode for the circular BNS merger at $R = 800 M_\odot$. Different lines compare the results of the different extraction algorithms: RWZ (solid blue), RWZ R-extrapolated (solid red), and CCE (dashed black). From top to bottom: amplitude and real parts, amplitude relative differences, and phase differences with respect to the CCE waveform.

the precursor; cf. Fig. 10. The extrapolated RWZ signal improves up to 3 orders of magnitude the amplitude relative differences.

Analogous results are obtained for the (2, 0) waveform of the pressure-perturbed TOV and for the BBH problem. In the latter case, we observe ~ 1 order of magnitude improvement in the agreement between RWZ and CCE.

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