High-accuracy gravitational waveforms for binary black hole mergers with nearly extremal spins

Geoffrey Lovelace\textsuperscript{1}, Michael Boyle\textsuperscript{1}, Mark A Scheel\textsuperscript{2} and Béla Szilágyi\textsuperscript{2}

\textsuperscript{1} Center for Radiophysics and Space Research, Cornell University, Ithaca, NY 14853, USA
\textsuperscript{2} Theoretical Astrophysics 350-17, California Institute of Technology, Pasadena, CA 91125, USA

E-mail: geoffrey@astro.cornell.edu, boyle@astro.cornell.edu, scheel@tapir.caltech.edu and szilagyi@tapir.caltech.edu

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Abstract

Motivated by the possibility of observing gravitational waves from merging black holes whose spins are nearly extremal (i.e. 1 in dimensionless units), we present numerical waveforms from simulations of merging black holes with the highest spins simulated to date: (1) a 25.5-orbit inspiral, merger and ringdown of two holes with equal masses and spins of magnitude 0.97 aligned with the orbital angular momentum; and (2) a previously reported 12.5-orbit inspiral, merger and ringdown of two holes with equal masses and spins of magnitude 0.95 anti-aligned with the orbital angular momentum. First, we consider the horizon mass and spin evolution of the new aligned-spin simulation. During the inspiral, the horizon area and spin evolve in remarkably close agreement with Alvi’s analytic predictions, and the remnant hole’s final spin agrees reasonably well with several analytic predictions. We also find that the total energy emitted by a real astrophysical system with these parameters—almost all of which is radiated during the time included in this simulation—would be 10.952\% of the initial mass at infinite separation. Second, we consider the gravitational waveforms for both simulations. After estimating their uncertainties, we compare the waveforms to several post-Newtonian approximants, finding significant disagreement well before merger, although the phase of the TaylorT4 approximant happens to agree remarkably well with the numerical prediction in the aligned-spin case. We find that the post-Newtonian waveforms have sufficient uncertainty that hybridized waveforms will require far longer numerical simulations (in the absence of improved post-Newtonian waveforms) for accurate parameter estimation of low-mass binary systems.

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(Some figures may appear in colour only in the online journal)
1. Introduction

In the next decade, advanced ground-based detectors such as the advanced Laser Interferometer Gravitational-Wave Observatory (advanced LIGO) [1, 2], Virgo [3] and the Large-scale Cryogenic Gravitational-wave Telescope (LCGT) [4] are expected to directly observe gravitational waves for the first time; coalescing black holes are among the most important sources of gravitational waves for these detectors. Numerical predictions of binary black hole (BBH) waveforms are crucial tools for detecting these waves: for example, the Numerical INJection Analysis (NINJA) project [5, 6] is testing gravitational-wave search pipelines using numerical BBH waveforms and the Numerical-Relativity and Analytical-Relativity (NR-AR) project [7] is working to calibrate analytic template banks for gravitational-wave searches using numerical BBH waveforms. Numerical BBH waveforms are also important tools for parameter estimation [8–11]. On the other hand, numerical simulations alone are too costly to provide all the information needed for detection and parameter estimation; the results must be combined with post-Newtonian (pN) approximations [12–14].

Beginning with Pretorius’s 2005 breakthrough [15], several groups have successfully completed numerical simulations of the inspiral, merger and ringdown of BBHs in a variety of configurations (see [16, 17] for recent reviews). Simulations of BBHs with merging holes whose spins are nearly extremal (i.e. \( \sim 1 \) in dimensionless units, the theoretical upper limit for stationary holes) are a challenging but potentially important case, since black holes with nearly extremal spin might exist [18–26] and thus might be among the BBHs emitting gravitational waves. Almost all published BBH simulations to date start with initial data in which three of the four Einstein constraint equations are solved analytically using the solutions of Bowen and York [27, 28]; this choice of initial data limits the black-hole dimensionless spins to \( \chi \lesssim 0.93 \) [29–31]. Dain, Lousto and Zlochower have closely approached this ‘Bowen–York limit’ by evolving an equal-mass BBH with equal spins of magnitude \( \chi = 0.924 \) aligned with the orbital angular momentum [32]. Note that the Bowen–York limit is actually far from extremal in terms of the physical effects of the spin: for example, a black hole with spin \( \chi = 0.93 \) has only 59% of the rotational energy\(^3\) of an extremal hole of the same mass.

By using an alternative method to construct BBH initial data, one can surpass the Bowen–York limit. In [34], three of us (Lovelace, Scheel and Szilágyi) constructed and evolved (through 12.5 orbits, merger and ringdown) BBH initial data (based on a weighted superposition of two boosted, spinning Kerr–Schild black holes [35]) with equal masses and equal spins of magnitude \( \chi = 0.949 \) anti-aligned with the orbital angular momentum. In this paper, we present a new BBH simulation (through 25.5 orbits of inspiral, merger and ringdown) with spins of magnitude \( \chi = 0.969 \) aligned with the orbital angular momentum. These simulations are the first to surpass the Bowen–York limit and contain the most nearly extremal black holes yet simulated, with the black holes with spin \( \chi = 0.949 \) and \( \chi = 0.969 \) having 65% and 72% as much rotational energy, respectively, as an extremal hole of the same mass.

In this paper, we consider the gravitational waveforms from these two simulations. We begin in section 2 by summarizing the numerical methods we use to construct and evolve rapidly spinning BBH initial data and also the methods used to extract and extrapolate the gravitational waveforms. In section 3, we examine the horizon mass and spin evolution in the new \( \chi = 0.969 \) simulation. Then, in section 4.1, we examine the emitted gravitational waveforms and their accuracy. In section 4.2, we compare the numerical waves to several

\(^3\) The rotational energy of a Kerr black hole is defined as the difference between its mass \( M \) and its irreducible mass \( M_{\text{irr}} := \sqrt{A/16\pi} \), where \( A \) is the horizon area; this is the amount of energy that can be extracted from a black hole. For details, see, e.g., the discussion in chapter 25 of [33].
The evolution (but not the properties of the resulting gravitational waveform) of configuration $S_{++}^{0.97}$ was first reported in [34]; we present the evolution of configuration $S_{++}^{0.97}$ for the first time.

### 2. Numerical methods

#### 2.1. Initial data

To construct BBH initial data with rapid spins, we use the method of [35] and the references therein: we use a spectral elliptic solver [37] to solve the extended conformal thin sandwich equations with quasi-equilibrium boundary conditions [38–43]. We choose free data based on a superposition of two boosted, spinning Kerr–Schild black holes, tuning the freely specifiable parameters with a numerical root-finding algorithm based on Broyden’s method [44, 45] to obtain the desired masses and spins. We reduced the orbital eccentricity using the iterative technique of [46] which is based on fits of the orbital frequency.

We summarize the two configurations we consider in tables 1 and 2.

#### 2.2. Evolution

We evolve the initial data summarized in the section 2.1 using the spectral Einstein code (SpEC) using the methods summarized in section III of [34], which extend the techniques of [47] and the references therein to accommodate BBHs with spins above the Bowen–York limit. The evolution (but not the properties of the resulting gravitational waveform) of configuration $S_{++}^{0.95}$ was first reported in [34]; we present the evolution of configuration $S_{++}^{0.97}$ for the first time.
here. Full details of our methods will be given in a future paper; here, we merely summarize our method, highlighting some of the additional techniques necessary to merge $S_{0.97}^{++}$. As described in [34], we excise the singularities inside the black holes from our computational domain, using a time-dependent, adaptively adjusted coordinate mapping to keep the excision surfaces inside the horizons. Because we do not apply boundary conditions on the excision surface, the evolution is only well-posed if the excision surface is a pure-outflow surface (i.e. if it has no incoming characteristic fields). During the inspiral, we enforce this condition by controlling the size of the excision surface such that it tracks the size of the apparent horizon; shortly before merger (i.e. during the final $\sim 1$ orbit of evolution $S_{0.95}^{--}$ and during the final $\sim 3$ orbits in the evolutions of $S_{0.97}^{++}$), we control the characteristic speeds directly by adjusting the velocity of the excision surface. During the final $\sim 0.25$ orbits before merger of $S_{0.95}^{--}$ and during the final $\sim 3$ orbits in $S_{0.97}^{++}$, we employed the spectral adaptive mesh refinement summarized in [34]. We also note that when evolving both $S_{0.95}^{--}$ and $S_{0.97}^{++}$, we smoothly change gauge conditions from that of the quasi-equilibrium initial data to the damped-harmonic condition described in [47] at the beginning of the evolution (instead of shortly before merger).

Because the holes spend more time in a highly dynamical and distorted state, we find that merging $S_{0.97}^{++}$ requires that our coordinate mapping must track the apparent-horizon shapes more accurately (i.e. to a higher spherical-harmonic resolution $\ell$). We also find that we must carefully fine-tune the characteristic speed control to balance two competing requirements: (1) that the excision surface has no incoming characteristic fields and (2) that the excision surface remains inside the apparent horizon. Here, we do this fine-tuning manually in order to merge $S_{0.97}^{++}$; in the future, we plan to employ a method that handles any tuning automatically. Because the remnant hole also has a rapid spin (particularly just after it forms (figure 2)), we similarly control the horizon shape and characteristic speeds during the ringdown of $S_{0.97}^{++}$ (with some manual fine-tuning).

To measure the characteristic speeds on the excision surface with sufficient accuracy near merger, just before merger in $S_{0.97}^{++}$ we adopt a computational domain where the individual apparent horizons lie within a thin, high-resolution spherical shell (instead of within a set of cylindrical subdomains, as evolution $S_{0.95}^{--}$ employed).

The right panel of figure 1 shows the numerical convergence of our method for the more demanding case $S_{0.97}^{++}$. The constraints initially grow, and then drop as the initial burst of spurious gravitational radiation leaves the computational domain. The constraints then remain clearly convergent throughout the inspiral. Shortly before enabling spectral adaptive mesh refinement, we found it necessary to increase the resolution of the inner spheres in the low-resolution run in order to control adequately the characteristic speeds; this appears as a discontinuous drop in the low-resolution constraint energy. As the evolution approaches merger, the constraint violation grows in spite of the spectral adaptive mesh refinement. During ringdown, the constraints rapidly drop as the hole relaxes to its final state. As the radiation leaves the grid, the constraints drop sharply in the low and medium resolutions but not in the high resolution.

Finally, we briefly note the computational cost of these two runs. Because the $S_{0.97}^{++}$ simulation involves higher spins, a very large orbital hangup effect (requiring twice as many

4 After a common horizon forms, our numerical simulation stops, interpolates onto a new computational domain with only a single excised region just inside the common horizon, and then continues using this new domain. Thus, the numerical resolution used during the ‘plunge’ (i.e. just before merger) is different from during the ‘ringdown’ (i.e. just after merger). The lack of convergence at late times in figure 1 follows from differences in the medium and high plunge resolution. All three plunge resolutions required different fine-tuning in order to merge; we presume that these differences are responsible for the behavior visible in figure 1. We have verified that for the highest plunge resolution, the constraints converge with the ringdown resolution, even at late times.
orbits to merge from the same initial separation as the $S_{0.95}$ simulation) and a large amount of time in a regime where the spacetime is highly dynamical, the $S_{0.97}^{++}$ simulation turned out to be much more computationally expensive than the $S_{0.95}^{−−}$ simulation. Specifically, the high-resolution simulation $S_{0.97}^{++}$ required $\approx 110,000$ cpu hours ($\approx 120$ days of wallclock time). For comparison, the high-resolution $S_{0.95}^{−−}$ simulation required $\approx 20,000$ cpu hours ($\approx 20$ days of wallclock time).

2.3. Waveform extraction

We extract the gravitational waveform $h$ using the Regge–Wheeler–Zerilli formalism [49–52] on concentric spheres with radii from roughly $r = 100–400M$; we then extrapolate the waveforms to infinite radius using the method of Boyle and Mroué [54] with polynomials of order $N = 4$. The waveforms are decomposed in the standard way [55] as modes $h_{\ell,m}$ of spin $s = −2$ spherical harmonics. We use these modes to define the amplitude and phase of the waveforms in the usual way:

$$A_{\ell,m}(\tau) = |r h_{\ell,m}(\tau)/M| \quad \phi_{\ell,m}(\tau) = \text{unwind}[\arg[h_{\ell,m}(\tau)]]$$

(1)

where the factor of $r/M$ removes the radial dependence from $A_{\ell,m}$ and the unwind function removes discontinuities of $2\pi$ in the data caused by branch cuts [56]. We also use the frequency $\omega_{\ell,m}(\tau) = \partial_\tau \phi_{\ell,m}(\tau)$. We will occasionally drop the subscripts on these quantities, implicitly referring to $(\ell, m) = (2, 2)$.

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5 We extract at finite radii and then extrapolate, since our computational domain only extends out to some finite radius. Extrapolation is meant to eliminate near-field effects and gauge dependence; to verify that the extrapolated waves do not retain any residual gauge dependence, the extrapolated waves could be compared with waveforms obtained using Cauchy characteristic extraction (CCE; see [53] and references therein for details). In the future, we plan to compare CCE waveforms with the extrapolated waveforms presented in this paper.
3. Mass and spin evolution in the $S_{0.97}^{+}$ simulation

In figure 2, we show the dimensionless spin (measured using the quasilocal, approximate Killing vector method described in appendix A of [35]) as a function of time for each resolution of the $S_{0.97}^{+}$ simulation. During the initial relaxation, the holes absorb energy, causing the dimensionless spin to quickly relax from $\chi = 0.9700$ at time $t = 0$ to $\chi = 0.9695$ at time $t = 1000 M$.

Similarly to [32], we observe a very large orbital hangup [59, 62, 63] during the long inspiral: starting from the same initial coordinate separation (and thus at approximately the same initial orbital frequency), case $S_{0.97}^{+}$ requires more than twice as many orbits to merge as does the case $S_{0.95}^{-}$ (compare the left panel of figure 1 and the top-left panel of figure 3 in [34]) and reaches roughly twice the orbital frequency. During this long inspiral, the spin remains above $\chi = 0.969$ during the first 21.5 orbits but then decreases near merger as the spin angular momentum is transformed into orbital angular momentum via tidal interactions.

The mechanism by which this transformation of angular momentum takes place has been described by numerous authors [64–68] including Alvi [36], who gave expressions for the rate at which energy and angular momentum would be transferred in comparable-mass binaries. In figure 3, we plot those rates as measured in the $S_{0.97}^{+}$ simulation and compare to those predicted by Alvi. Alvi’s expression uses the pN velocity parameter $v$ which we set to $v = (M \Omega)^{1/3}$, where $\Omega$ is the orbital angular frequency measured in the simulation. Though this comparison is gauge dependent, we find very good agreement—within the numerical uncertainty until very late in the simulation. A similar comparison for the $S_{0.95}^{-}$ case is not as useful because

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6 We infer the orbital frequency from the time-dependent, dynamically adjusted coordinate mapping that we use to keep the excision surfaces inside the apparent horizons; specifically, we infer the orbital frequency from the portion of this mapping that tracks the rotational motion of the horizons.
the numerical uncertainties are far larger though the result is consistent within the larger uncertainties. Note that this transfer of angular momentum is a 2.5-pN spin effect which is incorporated into the calculation of the pN waveforms in section 4.2.

When the common apparent horizon first forms, its spin is very nearly extremal but then quickly relaxes as the common horizon expands, increasing its area and eventually settling to a final spin \( \chi_{\text{final}} = 0.94496 \pm 0.00001 \), which is roughly consistent with the predictions of several analytic approximations (right panel of figure 2). We have verified that the common horizon is subextremal in the sense that it satisfies the inequality (equation (19) of [69])
\[
q := \frac{S}{2M_{\text{irr}}^2} < 1,
\]
where \( M_{\text{irr}} := \sqrt{A_{\text{AH}}/(16\pi)} \) is the irreducible mass and \( A_{\text{AH}} \) is the horizon area. Both \( q \) and \( \chi \) are nearly unity when the common apparent horizon first forms and then sharply decrease as the horizon area increases. As Booth and Fairhurst note in [69], there is no proof that non-Kerr black holes should satisfy this inequality; nevertheless, the inequality appears to hold in simulation \( S_{0.97}^{++} \). While this observation motivates us to conjecture that the common horizon in BBHs will always be subextremal (just as the initial data method we adopt appears incapable of generating super-extremal black holes [35]), we have no proof, and we cannot rule out the possibility that future BBH simulations at even higher spins might yield super-extremal common horizons or even naked singularities. We plan to test our conjecture in the future by exploring numerical simulations of merging black holes with even higher spins.

The mass of the final hole is \( M_{\text{final}}/M = 0.89048 \pm 0.00002 \). Alvi’s formulas suggest that the mass would change by less than a part in \( 10^8 \) prior to the beginning of our simulation if the binary had inspiraled from infinite separation; therefore, a ‘real’ binary would have radiated \( E_{\text{rad}}/M = 1 - M_{\text{final}}/M = 10.952\% \pm 0.002\% \) of its initial mass (\( = 12.299\% \pm 0.003\% \) of its final mass) throughout its entire inspiral, merger and ringdown. This efficiency is comparable to but larger than the predictions given by the analytic formulas in [57] (7.4\% \pm 1.4\%), [59] (7.9\%), [61] (9.7\%) and [70] (9.7\% \pm 0.1\%). The efficiency of the energy radiated by the \( S_{0.97}^{++} \) BBH is comparable to the efficiency of a supernova (\( \approx 15\% \) of the final core mass radiated;
see, e.g., equation (18.1.1) of [71]) but corresponds to a larger total energy radiated (since the mass of a BBH is typically larger than the final core mass after a supernova). For comparison, the simulation in [72] implies that an equal-mass nonspinning binary system would radiate about 5% of its mass, while table 1 shows that the $S^0_{0.95}$ system radiates about 3.17% of its mass. When the merger occurs at a frequency in the sensitive band of a gravitational-wave detector, we can therefore expect that an aligned-spin system should have significantly larger SNR than a similar system with anti-aligned spins.

4. Gravitational waveforms and pN comparisons

To compare two waveforms, $A$ and $B$, we need to align them by fixing the arbitrary relative time and phase offsets. Here $A$ and $B$ may refer to two numerical waveforms with different resolutions or extrapolation orders, or $A$ and $B$ may refer to pN and numerical waveforms. Following [73], we align the waveforms by minimizing the difference in their phases over a certain range. Specifically, we minimize\(^7\) the quantity

$$ \mathcal{E}(\Delta t, \Delta \phi) = \int_{t_1}^{t_2} \left[ \phi_A(t) - \phi_B(t - \Delta t) - \Delta \phi \right]^2 \, dt. $$

Each mode of waveform $B$ is then transformed as

$$ h_{\ell,m}(t) \rightarrow h_{\ell,m}(t + \Delta t) \, e^{-im \Delta \phi/2}. $$

Note that $\phi$ refers to the phase of the $(\ell, m) = (2, 2)$ mode only; the values of $\Delta t$ and $\Delta \phi$ are determined once, and then each mode is transformed by this equation.

The optimal values of $\Delta t$ and $\Delta \phi$ determined by minimizing equation (2) clearly depend on the range of integration $(t_1, t_2)$. We choose that range based on the frequencies of the waveform [10] so that $\omega(t_1) \approx 0.033$ and $\omega(t_2) \approx 0.038$.\(^8\) This gives us a common basis for comparison of the ranges used in the two cases of aligned and anti-aligned spins, despite the very different lengths of time over which they inspiral.

4.1. Waveform accuracy

We plot the amplitudes of the three dominant modes and the phase of the dominant $(\ell, m) = (2, 2)$ mode in the upper panels of figure 4 (for $S^0_{0.97}$) and figure 5 (for $S^0_{0.95}$). We also estimate the accuracy of the waveforms by measuring convergence with respect to increasing numerical resolution in the simulations and with respect to increasing order of the polynomial used for extrapolation to infinite radius. The relative amplitude convergence and phase convergence are plotted in the lower panels of the two figures.

The overall uncertainty estimate for a given quantity is the sum of the absolute values of the resolution convergence and the extrapolation convergence. That is, in the notation of the figures, we estimate

$$ \text{Uncertainty} \approx |(\text{Med.}) - (\text{High})| + |(N = 4) - (N = 3)|. $$

For a waveform to be included in the NINJA-2 data set [5], the amplitude and phase of the (2, 2) mode must be accurate at merger to within 5% and 0.5 rad, respectively. The $S^0_{0.95}$ case exceeds these requirements. The $S^0_{0.97}$ case, however, exceeds the amplitude requirement but

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\(^7\) For fixed $\Delta t$, the optimal $\Delta \phi$ can be obtained analytically, reducing the minimization to a one-dimensional problem. See [73] for details.

\(^8\) This range corresponds to $\delta \omega/\omega \approx 15\%$, which is somewhat larger than the 10% minimum recommended by MacDonald et al [10]. We use a larger range to ensure that the alignment is not skewed by small oscillations in the data.
Figure 4. The extrapolated gravitational-wave amplitudes and phase for simulation $S^{0.97}_{+}$: Left: the dominant wave amplitudes $A_2$, $A_3$ and $A_4$ at high resolution (top) and relative differences $|\delta A_2/A_2|$ between resolutions or between extrapolation orders (bottom). Right: the phase $\phi$ at high resolution (top) and differences $|\delta \phi|$ between resolutions (bottom). When computing differences, the waveforms are aligned as in (2) between $(t-r_*)/M = 1322$ and $(t-r_*)/M = 2852$. The merger time $(t-r_*)/M = 6411$ is the time at which the $2,2$ amplitude is maximal, denoted by the vertical dashed lines. If the waveform were instead truncated to five orbits before the merger (the NINJA-2 length requirement), the amplitude and phase errors would drop significantly (dotted lines). Note that the scale on the horizontal axis changes at $(t-r_*)/M = 6000$ in each plot for improved visibility of the merger and ringdown.

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does not meet the phase accuracy requirement. Through the time of merger, the amplitude uncertainty never exceeds 2%, but the phase uncertainty at the time of merger is 0.9 rad.

While the complete $S^{0.97}_{+}$ waveform does not meet the NINJA-2 accuracy requirement for the phase, this simulation’s 25.5 orbits far exceed the NINJA-2 length requirement of five orbits aligned with pN before a frequency of $M \omega = 0.075$. Indeed, if we omit the first 5000 $M$ of the $S^{0.97}_{+}$ waveforms, the simulation still easily meets the length requirements. Evaluating the errors by aligning between the beginning of the shortened waveforms and $M \omega = 0.075$, the convergence measure improves by a factor of 10, and the simulation comfortably exceeds the NINJA-2 accuracy requirements with a phase uncertainty of 0.1 rad at the time of merger, as shown by the dotted lines in the lower panels of figure 4. Thus, we see that using accuracy requirements of this sort without regard to the length of the simulation actually creates a perverse incentive to produce shorter numerical waveforms, which decreases the accuracy of complete ‘hybridized’ waveforms [11]. An exactly analogous situation occurs when the criteria require a particular match with respect to a detector noise curve but do not stipulate a mass at which that match should be measured; again, the incentive is to produce shorter waveforms. One way to avoid these incentives in future studies like NINJA would be to scale the required phase error with the length of the numerical waveform. However, such an improvement would still fail to describe the effect that errors in the simulation would have on the final results of the analysis. In particular, hybrid waveforms based on simulations of identical length and accuracy could still have radically divergent total accuracies, due to variations in pN accuracy for systems with different parameters. Ideally, accuracy criteria would be based on the impact on the final results, as suggested in [11].

$$\frac{\delta A_2}{A_2} = 10^{-2}$$

$$\frac{\delta \phi}{\phi} = 10^{-3}$$

$$\frac{\delta A_2}{A_2} = 10^{-3}$$

$$\frac{\delta \phi}{\phi} = 10^{-4}$$

$$\frac{\delta A_2}{A_2} = 10^{-4}$$

$$\frac{\delta \phi}{\phi} = 10^{-5}$$
4.2. Comparison with pN approximations

The pN waveform is constructed in two steps: (1) computation of the orbital phase of the binary and (2) computation of the amplitude of the waveform using that phase. For nonspinning systems, the formulas needed for those computations have been calculated to the 3.0 pN order beyond the leading order in amplitude and 3.5 pN beyond the leading order in phase. Additional spin–orbit and spin–spin terms are available to 3.0 pN order in phase and amplitude\(^9\), though not all of these have yet been expressed in a useful form for generating waveforms. We use the expressions given in appendix 1 of [55] for the flux, orbital energy and tidal heating, and the expressions given in equation (9.4) of [75] and appendix 2 of [55] for the waveform amplitudes. The sole addition we make is the inclusion of a recently published spin–orbit contribution to the flux. In [55], equation (A.13) should be supplemented by adding a term [74] as

\[
\mathcal{F}(v) \rightarrow \mathcal{F}(v) + \frac{32}{5} v^{10} \eta^2 \left[ v^6 \left( \frac{\pi}{6} (65 \delta \chi_a + (65 - 68 v) \chi_s) \right) \right].
\]

Though formally high in order, this term is large enough in magnitude (for the spins we present) to dominate the next-to-leading order spin contribution to the flux during most of the simulations, dominating even the leading-order term several hundred \(M\) before merger.

The orbital phase is computed using an energy-balance equation incorporating the rate of change of orbital energy and the loss of that energy in the form of tidal heating and the gravitational-wave energy flux \(\mathcal{F}\). Various methods exist—referred to as the TaylorT1, T2, T3 and T4 approximants [76, 77, 56]—for integrating these equations, all of which should be equivalent to the pN order available, in the sense that they differ only by higher-order pN terms. This suggests that all four approximants should agree with each other and with the

\(^9\) See [74] and references therein.
numerical waveform, within the uncertainty of the pN approximations. We have re-derived each of these approximants using the expressions described above and compared the results of each to the numerical waveforms.

Figures 6 and 7 show the pN comparisons for $S^{0.97}_{++}$ and $S^{0.95}_{--}$, respectively. Only the phase of the $(2, 2)$ mode is shown, because the phases of other modes are integer multiples of this
to a good degree of accuracy. The gray region in the background of each plot shows our uncertainty estimate for the numerical data of the given quantity, given by equation (4), and made to be a non-decreasing function of time after the beginning of the alignment region.

One remarkable feature is that the TaylorT4 approximant captures the phase surprisingly well for the \( S_{1+}^{3.97} \) system (black line in the top-left plot of figure 6); it agrees with the numerical data within the uncertainty for roughly 3400\( M \) after the end of the alignment region (in which it is forced to agree with the numerical data). This brings it within 200\( M \) of the merger. Contrast that agreement with the other approximants, which disagree with the numerical data immediately after (or even before) the end of the alignment region.

Of course, this agreement of TaylorT4 is presumably pure coincidence, as all approximants agree with each other within the uncertainty of the pN approximations. The same coincidence was found in the equal-mass nonspinning case [56], but has been shown not to carry over to systems with other parameters (see, e.g., [63]). Indeed, looking at the to which the amplitudes are known decreases with increasing accurate, becoming worse for higher modes. This is to be expected, as the relative pN order [82, 83]. For stronger signals or lower masses, more accurate pN waveforms and in these hybrids would be larger than the statistical uncertainty due to noise in the detector immediately after (or even before) the end of the alignment region.

Contrast that agreement with the other approximants, which disagree with the numerical data of the pN approximations for the amplitudes of the three dominant modes. In each case, the amplitude of the \((\ell, m) = (2, 2)\) mode is the most accurate, becoming worse for higher modes. This is to be expected, as the relative pN order to which the amplitudes are known decreases with increasing \( \ell \). In particular, the \((2, 2)\) mode is known to relative 3 pN order, while the \((3, 2)\) and \((4, 4)\) modes are only known to relative 2 pN order. Nonetheless, because of their far smaller magnitude, these higher-order modes actually have comparable absolute accuracy.

The \((3, 2)\) mode is particularly interesting. In the \( S_{1+}^{3.97} \) case, its amplitude is comparable to that of the \((4, 4)\) mode. However, in the \( S_{1+}^{3.95} \) case, the \((3, 2)\) mode is much smaller until the merger. For most of the inspiral, the pN amplitude error is very large—being off by roughly 80\%. Again, however, this error is relative; the pN approximation correctly predicts that the amplitude should be quite small in this case because of a cancellation between the leading-order nonspinning and spinning components of the amplitude.

Finally, we note that both waveforms can be hybridized to pN waveforms at frequencies of \( M \omega \approx 0.035 \), though these hybrids are not necessarily accurate enough to be useful in parameter estimation for detector-data analysis. As in [11], we can estimate the error in any hybrid by measuring the mismatch [78–80] between each pair of hybrids formed with the various approximants TaylorT1–T4; the error estimate is the maximum such mismatch. Using the Advanced LIGO high-power noise curve with no detuning [81] to do this measurement for the \( S_{1+}^{3.97} \) system, we find mismatches larger than 0.01 for total masses below roughly 40\( M_{\odot} \). This means that for any detected (SNR \( \gtrsim 8 \)) system with a lower mass, the uncertainty in these hybrids would be larger than the statistical uncertainty due to noise in the detector [82, 83]. For stronger signals or lower masses, more accurate pN waveforms and/or longer numerical simulations would be needed. For the \( S_{1+}^{3.95} \) case, a similar comparison would lead us to conclude that the hybrid is completely uncertain because of the bad behavior of the

\[ \text{To be more precise, the TaylorT3 approximant expresses the orbital frequency of the binary as a function of the pN time to coalescence by inverting a power series (which is used directly for the TaylorT2 approximant). Because of logarithmic terms, this inversion is not directly well-posed at high pN order; the logarithmic terms must be arbitrarily set to constants for the inversion [14]. The resulting frequency never reaches the initial frequency of our simulation, the frequency plot ‘turns over’ before that point. This is not unusual behavior for TaylorT3. For example, even in the nonspinning case, similar behavior is seen for mass ratio 10:1. These results suggest that the TaylorT3 approximant may be particularly unreliable.}\]
TaylorT3 approximant. If, on the other hand, we exclude that approximant as anomalously bad, we find that the hybrids are only accurate enough for parameter estimation above roughly $60M_\odot$. Still it is possible that such hybrids would be accurate enough for detection purposes [11, 84].

5. Conclusion

The simulations discussed in this paper contain the most nearly extremal BBHs simulated to date. In our spin 0.97 simulation, we have found remarkably good agreement between the horizons’ mass and spin evolutions and Alvi’s analytic predictions, but we have found only moderately good agreement between the remnant hole’s final spin and several analytic formulas, which suggests that these analytic formulas could be improved significantly using a set of aligned and anti-aligned nearly extremal BBH simulations.

We have found that the waveform from the 12.5-orbit anti-aligned case $S_{0.95}^-$ exceeds the NINJA-2 accuracy requirements, while the waveform from the 25.5-orbit aligned case $S_{1.07}^+$ exceeds the NINJA-2 amplitude requirement but (because it is so long) fails to meet the NINJA-2 phase requirement (although it does meet the phase requirement easily if truncated to five orbits, the NINJA-2 length requirement).

These results demonstrate the feasibility of applying waveforms from numerical simulations to gravitational-wave data analysis efforts when the holes have nearly extremal spins—a case previously inaccessible numerically but relevant astrophysically, given the evidence that nearly extremal black holes could exist. For example, waveforms such as those considered in this paper could be used in calibrating analytic template banks used for gravitational-wave detection searches. To pursue this goal, we plan to apply our methods for evolving nearly extremal BBHs to a large variety of BBH configurations, including unequal masses and spin precession.

We have compared our numerical waveforms to several pN approximants, finding that the pN and numerical waveforms disagree at times well before merger. We also find that the pN approximants disagree with one another, indicating a large uncertainty in the pN approximations which leads to a large uncertainty in the resulting hybridized waveforms. Similarly to the results of Hannam et al [85], we find that TaylorT4 approximates the phase of the waveform to high accuracy in the aligned-spin case, while TaylorT1 is best in the anti-aligned-spin case. However, we also find that a recently published [74] spin–orbit contribution to the flux (equation (5)) contributes a very large portion of the effect of spin and is crucial to the accuracy in both cases.

Extracting the BBH parameters from detector data for systems with nearly extremal spins will require far longer numerical simulations, far more accurate pN waveforms or a combination of the two. In the absence of improved pN waveforms, however, this implies that parameter estimation when the holes have nearly extremal spins could prove quite challenging, since the longer numerical simulations that would be necessary will come at high computational cost.

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