The current status of binary black hole simulations in numerical relativity

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Abstract
Since the breakthroughs in 2005 which have led to long-term stable solutions
of the binary black hole problem in numerical relativity, much progress has
been made. I present here a short summary of the state of the field, including
the capabilities of numerical relativity codes, recent physical results obtained
from simulations and improvements to the methods used to evolve and analyse
binary black hole spacetimes.

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1. Introduction

With the current generation of gravitational-wave (GW) interferometers (LIGO [1–3], Virgo
[4, 5], GEO [6–8] and TAMA [9]) reaching their design sensitivity, and the next generation
(Advanced LIGO [10] and LISA [11, 12]) planned to come online in the next few years,
the accurate modelling of GW sources and the construction of template waveforms to be
used in matched filtering of detector data has become urgent. One of the strongest expected
sources of gravitational waves is the inspiral and merger of a binary black hole (BBH) system.
Additionally, the modelling of BBH mergers has applications in astrophysics, where it can be
used to learn about possible growth methods for supermassive black holes, galaxy evolution
and globular clusters. BBH mergers occur in the regime of very strong gravity, and whilst
the early inspiral can be described accurately with approximate analytic post-Newtonian (PN)
methods, to model the late inspiral and merger requires the numerical solution of the Einstein
equations using expensive and complex supercomputer simulations in numerical relativity
(NR). Though the analytic framework and associated numerical simulations have been under
development since the 1960s, it was only in 2005 that simulations of multiple orbits of a BBH
system became possible. Since those first simulations [13–15], the quality of the computations
has improved significantly, and it is now possible to simulate enough orbits with a sufficiently
high accuracy that the resulting waveforms can be compared with PN results. NR waveforms

can be attached to PN waveforms to construct *hybrid* waveforms, fitted with *phenomenological* models, or used to tune effective-one-body (EOB) waveforms.

In this brief paper, I review recent developments in the field of numerical relativity. As such, this work is not intended to be a comprehensive discussion of the history of the subject. For more details on earlier work, particularly associated with waveforms for GW data analysis, see [16]. Several works had appeared while this manuscript was being prepared, and this demonstrates the healthy level of activity in the field. This paper is structured as follows. In section 2, I give a brief overview of the current capabilities of NR codes, including the longest waveforms and highest mass ratios studied so far. I also summarize the results of a validation study (the Samurai project) which verified the consistency of the waveforms produced by several codes in the community, and conclude the section with a discussion of some work on improvements to computational efficiency.

In section 3, I discuss new physics results which have been obtained using NR simulations, including comparisons with PN and EOB models. I then discuss some applications of NR to GW data analysis, including work on injecting numerical waveforms into data analysis pipelines (the NINJA project), the construction of phenomenological waveform templates and studies of NR results applied to the detection of gravitational waves and the estimation of the parameters of their sources. I then discuss the work that has been done on modelling the state of the final merged black hole as a function of the parameters of the initial black holes, as well as the work on hyperbolic (non-circular) and high-velocity BBH configurations.

In section 4, I present recent work on methods used in NR for BBH simulations. The proposed new techniques for generating improved initial data are reviewed, as well as work which has been done on boundary conditions. I then discuss studies involving the computation of gravitational waves from numerical simulations, including analyses of finite radius effects and extrapolation procedures, the asymptotic falloff of the Weyl scalars used for measuring spacetime content including gravitational radiation, and the first application of Cauchy-characteristic extraction (CCE) to produce unambiguous waveforms at future null infinity for BBH systems. I also discuss the development of new computational infrastructure for using non-Cartesian grids with finite differencing BBH codes, as well as improvements to the methods used for spectral BBH evolutions.

In section 5, I list the main challenges facing the NR community today, and present some closing remarks.

2. State of the art

There are now several groups around the world with codes capable of performing BBH simulations [13, 15, 17–26]. There are two analytic forms of the Einstein equations (BSSN [27–29] and generalized harmonic [13, 30, 31]), and various numerical methods (high-order finite differencing, pseudo-spectral, adaptive mesh refinement, multi-block) in use in the community.

2.1. Consistency

The gravitational waveforms computed by these codes for a given set of initial data should be independent of these differences as they represent a physical observable, so a comparison of the results of the different codes yields a strong test of consistency. The Samurai [32] project was a collaborative effort to compare the waveforms from five different codes for the last four orbits and merger of a binary of equal-mass, non-spinning black holes in a circular orbit. The codes were BAM [20], CCATIE [22], Hahndol [17, 33], MayaKranc [18]

and SpEC [21]. The first four use the BSSN formulation of the Einstein equations, though the coordinate conditions used are slightly different for each code. SpEC uses the generalized harmonic formulation. CCATIE and MayaKranc both use the same computational framework (Cactus/Carpet [34–37]), but the evolution and analysis codes are separate. The other codes used in the Samurai comparison are independent. SpEC uses a pseudo-spectral evolution scheme, whereas the others use finite differencing methods. Despite these differences, it was found that the waveforms all agreed with each other within their published error estimates. In GW data analysis, the quantity usually used to make comparisons between waveforms is the *match*, $\mathcal{M}$ [38]. This is a normalized frequency-domain scalar product of the waveforms, weighted by the detector noise, in the range zero to one, where a match of $\mathcal{M} = 1$ indicates two waveforms which are seen as the same by a given detector. We also refer to the *mismatch* $1 - \mathcal{M}$ of two waveforms. The mismatch between the Samurai waveforms was less than 10^{-3} for enhanced LIGO, Advanced LIGO, Virgo and Advanced Virgo, suggesting that the accuracy and consistency of the waveforms are sufficient for detection purposes. We should note here that, since only the last eight cycles of the waveform were considered, this result applies only to those systems where these cycles are the only ones in the detector bandwidth, i.e. those systems above a certain total mass. Also, only the dominant $l = 2$, $m = 2$ multipolar mode was considered, approximately corresponding to a system observed from a direction perpendicular to the orbital plane. The impact of the inclusion of higher modes and longer waveforms (e.g. constructed by joining NR to PN waveforms) in such a comparison has not yet been studied.

2.2. Longest waveform

The longest NR BBH waveform so far produced lasts for 15 orbits and includes the merger and ringdown phases, and is described in Boyle *et al* [39] and Scheel *et al* [40]. This waveform, from an equal-mass binary of non-spinning black holes, was generated using the SpEC code and, due to its length and quoted accuracy, has been used in a number of studies comparing NR and PN results [41–46]. This code uses a pseudo-spectral numerical method and multiple coordinate patches to cover the evolution volume and, in [47], new techniques were introduced which allow simulation of the full inspiral, merger and ringdown without the fine-tuning of parameters that was previously required. As a result of this work, simulations of BBH mergers with mass ratios $q = m_1/m_2 \geqslant 1$ (where $m_1 \geqslant m_2$ are the masses of the individual holes) of $q = 2$ and dimensionless spins up to 0.4 are now possible with the SpEC code, and these are presented in [47]. Additionally, simulations with dimensionless spins of 0.44 anti-aligned with the orbital angular momentum are presented in [48]. In a talk by Pfeiffer [49], a series of long unequal-mass simulations performed with the SpEC code was presented, with 15 orbits up to $q = 4$ and 8 orbits up to $q = 6$.

2.3. Highest mass ratio

For a 3D numerical relativity code, one of the most challenging problems is the simulation of black holes of very different masses. Unequal masses are expected to be commonplace astrophysically; hence, waveforms from these systems are essential. One early reason for the interest in unequal-mass BBH systems, besides the use of NR waveforms for GW science, was the fact that the mass asymmetry leads to an asymmetry in the linear momentum emitted in the gravitational waves around the merger, leading the final black hole to recoil out of the initial zero momentum frame. This recoil (also known as a *kick* or *rocket effect*), especially when the black holes are spinning, can have important consequences for astrophysics [50].

The highest mass ratio that has been simulated is $q = 10$. The first such simulation, reported in [51], consisted of three orbits of a binary of non-spinning black holes as well as the merger and ringdown of the final black hole to Kerr. The result was computationally very expensive to achieve, but it verified the prediction of the empirical recoil formula [52–54] in a range which had previously not been tested. The reason for the increase in computational expense is that, for a fixed total mass $M = m_1 + m_2$, the gravitational wavelength remains approximately constant with varying q, but the length and time scale required to resolve the smaller hole scales approximately with q. With adaptive mesh refinement as used in [51], for large q, the computational cost in CPU hours is q times higher than that for an equal-mass simulation. One technical problem which arises when simulating unequal-mass BBH systems relating to the coordinate conditions used in many codes has been studied recently in [55]. Due to the computational expense of simulating high mass ratios, it can be desirable to propagate the gravitational waves in a separate evolution. In [56], a BBH simulation with a mass ratio of 1:10 was presented, along with a computationally inexpensive perturbative evolution of the gravitational waves modelled using point particles as the sources, whose locations were determined from the coordinate tracks of the black holes in the numerical simulation.

2.4. Highest spin

Mathematically, Kerr black holes have a maximum dimensionless spin of 1, and there is a good probability that highly spinning black holes exist in nature [57–59]. Current NR techniques for simulating BBH systems are limited in the maximum spin which can be specified in the initial data, both for theoretical and numerical reasons. The common initial data formulations have mathematical limits on the spins which can be achieved (see section 4.1 for a discussion of techniques for constructing initial data with high spins). Numerically, black holes with high spins require more resolution and hence higher computational resources to achieve a given accuracy. Typically, black holes with dimensionless spins as high as 0.6–0.8 can be evolved with only a moderate increase in computational cost over the non-spinning case. However, the cost of simulating higher spins increases dramatically. For the Bowen-York initial data used by the majority of BBH codes, the theoretical maximum has almost been reached in [60], where ~ 7.5 orbits of black holes with dimensionless spins 0.92 are evolved. This is the highest spin so far for the inspiral-merger-ringdown of a BBH system simulated in NR.

2.5. Lowest eccentricity

BBH systems visible to GW detectors are usually expected to have circularized to an orbit of eccentricity zero due to the emission of gravitational radiation [61]. However, it is not known how to rigorously choose BBH initial data parameters so that the resulting orbit is quasi-circular. The lowest eccentricities have been obtained using a method presented in [62]. In this method, the first few orbits of a BBH evolution are performed and the initial data parameters are adjusted in an iterative procedure based on the measured eccentricity of the resulting evolution. With this method, eccentricities as low as $e \sim 5 \times 10^{-5}$ have been produced. This procedure must be repeated for every initial data set considered, though the computational cost is mitigated by the fact that the evolutions do not need a very high resolution. It should be noted that there is no fully general relativistic definition of eccentricity; definitions can be used which are based on the coordinate or proper separation of the black hole horizons, and these definitions are used in [62]. It would also be possible, though more difficult, to use the properties of the gravitational radiation, such as its amplitude or frequency.

2.6. Computational performance

As higher mass ratios and longer simulations are required, the performance of NR codes becomes more important. The XiRel project [63, 64] was started in order to improve the performance of the publicly available Carpet [36, 37] adaptive mesh refinement infrastructure. As a result of recent work, Carpet now scales efficiently up to 2048 processing cores, and as it is used for BBH simulations at AEI, GaTech, LSU, RIT and UIUC, the improvements benefit simulations by all of these groups.

3. New binary black hole physics

3.1. Comparisons with analytic models

Due to the high computational cost of NR BBH simulations, the early inspiral can instead be modelled using approximate analytic techniques based on the post-Newtonian method (see [65] for a recent review), and the late inspiral and merger can be simulated with NR. PN results are accurate in the regime where the black holes are far apart and moving slowly. For GW detection purposes, the use of longer waveforms increases the range of masses of systems which can be detected, so including the inspiral is very important. Recent work has focused on combining the waveforms from analytic methods with NR simulations to generate complete waveforms describing both the inspiral and merger. For a review of the first PN–NR comparisons see, for example, [16].

The effective-one-body (EOB) approach [66] (see [67] for a recent review) is heavily based on the PN method, but uses additional techniques to model the merger phase, which is usually inaccessible to PN methods. There are several unknown parameters in the various EOB methods, and these need to be determined by comparison with NR simulations. Two recent works, Damour *et al* [41] and Buonanno *et al* [42], have used the SpEC 15 orbit equal-mass, non-spinning waveform [39, 40] to tune the parameters in the EOB formalism, adding to the previous work on PN and EOB comparisons with this waveform in [43, 44]. After this tuning, the EOB model agreed with the NR waveform within the quoted numerical error on the NR waveform. For binaries with total masses between 30 and 150 $M_\odot$ (solar masses), there was a mismatch between NR and EOB of $<10^{-3}$ for LIGO, Enhanced LIGO and Advanced LIGO. This work was very recently extended in [46] to include the new SpEC waveform [48] incorporating spinning black holes.

In [68], a nine-orbit NR simulation of a configuration of spinning black holes of unequal mass with their spin axes misaligned with the orbital angular momentum was presented. This is the most general BBH configuration that can be expected in nature, assuming that such systems will have evolved to have zero eccentricity by the time the NR portion of the waveform enters the frequency range of GW detectors. The mass ratio was $q = 1.25$ and the dimensionless spins of the black holes were 0.6 and 0.4. In this simulation, significant precession of the orbit out of the initial orbital plane was observed, in agreement with PN spin–orbit and spin–spin coupling predictions (see, e.g., [69] for details). A comparison with 3.5 PN waveforms including spin effects was made, and the first six wave cycles (three orbits) agreed within 1% (note that this is a time-domain inner-product measure, not the conventional frequency-domain match $\mathcal{M}$ usually used in GW data analysis).

The work of Peters [61] in the 1960s demonstrated that a binary system in an eccentric orbit which is inspiralling due to the emission of gravitational radiation will lose eccentricity and eventually circularize. Typical GW sources are expected to circularize before they can be observed, so studies of sources of gravitational radiation usually assume circular

orbits. However, it has been suggested [70–74] that there may be sources with non-negligible eccentricity which are detectable by Advanced LIGO and LISA. In [75], the first comparison between an eccentric PN model and an NR simulation was performed. A ten-orbit simulation (20 GW cycles) with initial eccentricity $e \approx 0.1$ was presented, and an eccentric PN model was fitted to the resulting waveform. The two waveforms agreed within 0.1 radians for the first eight cycles, and by five cycles before the merger, a dephasing of 0.8 radians had occurred. Two different PN models were compared, and the choice of PN expansion variable was found to have a significant effect on the accuracy of the PN approximation.

3.2. Gravitational-wave data analysis

Due to the weak nature of gravitational waves, and the difficulties in separating GW signals from local vibrations, the output of ground-based GW detectors is dominated by noise. As a result, sophisticated statistical algorithms must be used to extract physical signals corresponding to the detection of gravitational waves from BBH systems. These algorithms, employing the technique of *matched filtering*, require accurate waveform *templates* corresponding to the sources to be detected.

For low mass systems (those with a total mass of between 2 and 35 $M_\odot$), current GW detector data is searched for signals using PN template waveforms. This is because for high masses, the GW frequency of the merger is too high to be seen by the detectors, whereas for low masses, pure PN templates can be sufficient [76]. Between 25 and 100 $M_\odot$, waveforms generated using the EOB formalism (not including spin effects) and tuned to NR (EOBNR [66, 77–79]) as well as phenomenological templates [80, 81] are currently used. For a recent status report on the searches of LIGO–Virgo data for signals from coalescing binaries, see [82], and for more information on the use of NR waveforms in GW data analysis, see [16].

Now that NR waveforms are available which include the merger phase, as well as a significant overlap with the regime of PN validity, it is important to test that the search algorithms work well with signals which include the merger. This work was started in the numerical injection analysis (NINJA) project [83–85]. The NR waveforms from ten different groups were injected into the data analysis pipeline software and the performance for detection and parameter estimation of these pipelines was characterized. The NR waveforms covered mass ratios up to $q = 4$, a range of spin configurations up to dimensionless spins of ∼0.9 and up to 30 GW cycles. The waveforms were converted into time-series data that would be seen at the detector and Gaussian noise, designed to mimic the features of each detector, LIGO, Virgo and Geo600, was added to the signal. Various data analysis techniques were then used to attempt to detect the signals in the data, and in some cases to estimate the source parameters. Overall, it was found that many of the current data analysis pipelines were able to detect the merger waveforms at the expected sensitivities, but that significant work is needed to improve parameter estimation. Additionally, the NINJA project has provided a working model for collaboration and communication between the NR and DA communities, which will be essential if the recent advances in NR are to contribute to GW science. The NINJA 2 project [85], which is currently underway, will incorporate hybrid waveforms (i.e. PN and NR waveforms combined), and real detector noise. This will allow stronger statements to be made concerning the performance of the detector pipelines for real signals.

In [86], a study was made of the signal to noise ratio (SNR) of a family of waveforms for BBH systems with spins aligned and anti-aligned with the orbital angular momentum. In this family, there is no precession of the orbital plane. It was found that the SNR increases with the projection of the total spin in the direction of the orbital angular momentum, and that if the spins are aligned with the orbital angular momentum and maximal (dimensionless spin

of 1), the SNR is three times as high as that in the anti-aligned case, leading to an increase in the event rate for current and advanced LIGO and Virgo detectors of a factor of $\sim$30. Hence, it is likely that there will be a bias in detected binaries towards high spins aligned with the orbital angular momentum, as these have the largest SNRs. It was also determined that the match between different cases is controlled by the total spin; binaries with zero total spin (including the case with both black holes non-spinning) are indistinguishable from each other (indicated previously in [18]) for LIGO, whereas binaries with a nonzero total spin have identifiably different GW signatures. This means that aligned spin detection templates only need a single spin parameter, which reduces the dimensionality of the search parameter space.

In [87], it is shown that if only non-spinning templates are used to search for signals from spinning systems, the event rate is reduced by up to 50%. To alleviate this problem, it is necessary to include spin effects in the templates used in GW data searches. The authors constructed time-domain hybrid waveforms by matching the waveforms from NR simulations covering at least eight waveform cycles to a PN approximant called *TaylorT1* [88]. Mass ratios up to $q = 3$ and dimensionless spins up to 0.85 aligned and anti-aligned with the orbital angular momentum were considered. Phenomenological Fourier-domain waveform models with free parameters were then constructed, and the parameters were fitted to the PN–NR hybrids. This resulted in a bank of template waveforms with freely adjustable mass ratio and spin parameters which can be used in a GW data-analysis pipeline, and should lead to higher detection rates for spinning BBH systems.

Once a detection has been made, the next step is to determine the parameters of the source, for example the sky location, mass ratio, total mass, etc. For the space-based detector LISA, the low noise levels mean that detection of BBH signals is generally not a problem; the challenge is to accurately determine the source parameters. In McWilliams *et al* [89], a comparison is made between the accuracy of parameter estimation when using purely PN waveform models and when using combined PN and NR models. It is found that the inclusion of the NR merger portion for supermassive BBH systems (for mass ratios $q < 10$) reduces the uncertainty in the sky-location of such a binary by a factor of $\sim$3 to within $\sim$10 arcmin.

3.3. Modelling the final state

Knowledge of the mass, spin and linear momentum of the final black hole in a BBH merger has many applications. One example is in the modelling of the evolution of cosmological black hole spins [90]. Another is in explaining the presence or absence of massive black holes in the centre of galaxies, as the merger of galaxies and their associated central massive black holes may result in recoils which eject the final black hole [50].

When it was predicted and then confirmed [91–93] that very large recoils could be generated in BBH mergers with specific spin orientations, a large amount of effort went into exploring this effect due to the potential application to astrophysics. Recently, in [94], the mass, spin and recoil velocity of the final merged black hole were modelled as functions of the spins just before the merger using expressions based on PN predictions, but with PN coefficients replaced by those obtained from fits to NR data. This is an extension of the previous work [53, 91, 95] including additional terms in the models. In [96, 97], the authors proposed formulae for properties of the final black hole (mass, spin, linear momentum) based on symmetry arguments and an expansion in the initial spin parameter. The final spin has more recently been addressed using an alternative approach (also see [98–100] for predictions based on point particles). In [101], following the work in [102–105], a set of approximations and simplifying assumptions is combined with a large body of already published NR data to produce a general formula for the spin magnitude and direction of the final black hole after

a merger. Instead of basing the model on PN expressions around the time of the merger, the final spin is expressed in terms of the spins early in the inspiral, and it is argued that this is more relevant when making astrophysical predictions, since an astrophysicist is not interested in the detailed dynamics of the merger, but instead in the final state obtained from a set of initial parameters when the black holes are far separated. In [106], PN evolutions and the empirical model of [95] are combined to make a link in a statistical sense between the early inspiral and pre-merger spins.

While the above works have concentrated on determining the final state of the black hole using empirical models, in [107], the dynamical momentum flow in the region near the black holes is studied. The method used is based on field theory on an auxiliary spacetime in which linear momentum is defined, and follows on from the previous work which treated the PN case [108]. In this way, the linear momentum of the individual black holes can be computed, albeit with some gauge dependence. It is found that, despite this gauge dependence, the linear momentum measured for a head-on collision of two black holes using this method agrees well between evolutions using different gauges, suggesting that this linear momentum measurement may have a physical interpretation.

3.4. Beyond circular inspirals

Due to its astrophysical importance, the BBH problem in NR is usually studied for quasi-circular configurations, i.e. those consisting of circular motion combined with a low inward radial velocity. However, there have recently been several works which studied non-quasi-circular configurations.

Hyperbolic BBH encounters can be thought of as orbits of eccentricity $e > 1$. In a Newtonian system, such a configuration would result in scattering of one black hole off the potential of the other, but in full GR, for a sufficiently small impact parameter, the black holes become gravitationally bound due to the emission of energy through gravitational waves and merge quickly [109]. In [110], it was found that hyperbolic encounters of spinning black holes resulted in a significant linear momentum imparted to the final black hole due to the asymmetry of the emitted radiation at the moment of the merger. Recoil velocities as high as $10\,000$ km s^{-1} could be obtained, in contrast with the quasi-circular case where the highest recoil velocity obtained is of the order of 3300 km s^{-1}. In [111], it was found that the final dimensionless spin could be as high as 0.98 when extrapolated to the case of maximally spinning black holes.

In particle physics, high energy collisions are used to probe the fundamental properties of nature. As these collisions are performed at higher and higher energies, it is expected that they will result in the formation of an event horizon, and that these scattering processes will be well modelled by the high velocity scattering of black holes. In [112], the authors studied high velocity head-on black hole collisions. The simulations included initial velocities up to $v = 0.94c$ and, when extrapolated to black holes moving at the speed of light, the energy radiated in the head-on collision was determined to be about 14%. In [113], the authors studied non-head-on high velocity collisions. By varying the angle of approach of the black holes, it was determined that the impact parameter should be approximately $b < 2.5GM/c^2/v$ for a black hole to form, where M is the total black hole mass. This model was fitted from the simulated velocities from $0.6c$ to $0.9c$. A similar study was performed in [114] where the result was confirmed for these velocities, but for higher velocity ($v = 0.94$), the formula in [113] may have been an overestimate.

Zoom–whirl orbits are characterized by quasi-circular motion (whirl), alternating with highly eccentric motion (zoom). For BBH systems, this phenomenon has been seen in extreme

mass ratio inspirals as well as PN models, and in [109] it was seen for the first time in NR. In [114], zoom–whirl behaviour is confirmed for the high velocity collisions studied, and in [115], the authors study zoom–whirl orbits for a variety of mass ratios and spins and show that they can occur without the need to fine-tune the initial data parameters. Furthermore, in [116], low momentum zoom–whirl orbits, expected to more closely reflect astrophysical scenarios, are simulated and the dependence of the energy radiated as a function of the initial angle of the black hole momenta is computed. They found that as the initial angle between the momenta and the coordinate line joining the two BHs increases from zero, there is a peak in the emitted energy at $47°$, followed by several local maxima.

3.5. Electromagnetic counterparts

Several recent works have studied possible electromagnetic (EM) signatures of BBH mergers. If such signatures are visible to current or future instruments, this opens up the possibility of coincident detection via EM and GW observations of BBH inspiral events. Not only might this increase the detectability of these events, but it might significantly increase the accuracy with which the parameters of the binary, such as the sky location and redshift, can be determined.

In [117, 118], the fully coupled Einstein–Maxwell system is evolved for an equal-mass, non-spinning BBH system in the presence of an external magnetic field but otherwise in vacuum. The system is designed to model the effect of the magnetic field sourced by an accretion disc around a supermassive black hole binary, where the matter from the accretion disc has been cleared from the immediate neighbourhood of the black holes by binary torques [119]. It is found that the EM fields evolve in a way which follows the dynamics of the binary and so they can be used as *tracers* of the motion. Additionally, the EM energy flux is found to oscillate with a quarter the orbital period of the binary and the energy in the EM field is found to increase as the binary approaches merger. For the astrophysically realistic field strengths used here, the addition of the EM field has no effect on the binary dynamics or waveform. Therefore, in the follow-up work by Mösta *et al* [120], the EM fields are treated as test fields and their evolution does not feed back into the evolution of the geometry. Here, larger initial black hole separations are used along with black hole spins aligned and anti-aligned with the orbital angular momentum. It is found that for the lowest multipolar modes, the EM radiation follows very closely the amplitude and phase evolution of the GW radiation, so that detecting either one gives direct information about the other. Furthermore, the EM energy flux scales quadratically with the black hole spin, and is 13 orders of magnitude lower than the GW energy flux. Most importantly, the frequencies of the EM radiation are well outside the range of existing radio observations and hence direct observation is highly unlikely.

In an alternative picture of the late inspiral of a supermassive black hole system, if the surrounding gaseous environment is sufficiently hot, as for example in the nuclear regions of some low luminosity active galactic nuclei (AGNs), there could be gas present near the black holes all the way up to and through the merger [121]. In [122], first steps are taken towards adding a gas into their BBH simulations by computing geodesics of the spacetime, and considering these to represent flows of test particles on the background geometry of the BBH solution. Differences in the collision and outflow speeds of the test particles are observed between single black hole and BBH systems, and between spinning and non-spinning black holes in binaries. In [123] and, independently, in [124], a supermassive BBH system is simulated in the presence of a gas modelled using full GR hydrodynamics. In [124], the rate of accretion of the gas onto the black hole is computed, and it is found that the luminosity of the resulting EM radiation is enhanced significantly over that expected from a single black

hole, and estimates of detectability of this radiation are given. In [123], correlations are found between the EM and GW emission. For the most massive supermassive black hole systems that would be detectable by LISA, the EM luminosities are here found to be high enough to be accessible to observations out to a redshift of $z \approx 1$ using x-ray measurements.

4. New binary black hole methodology

4.1. Initial data

Specification of initial data for a BBH evolution is a nontrivial task as this data must satisfy the Einstein constraint equations. These equations are nonlinear so it is not in general possible to construct initial data by superposing two single black hole solutions. There are two main methods for constructing BBH initial data in use for NR evolutions: Bowen-York puncture data [125, 126] and a method based on the conformal thin sandwich (CTS) decomposition of the equations involving excision of the black hole interiors from the domain [62, 127–130]. In both these cases, very roughly speaking, one chooses the desired characteristics of the black holes and then solves a set of elliptic equations numerically. Both of these methods are subject to several problems: incorrect initial radiation content, difficulty in controlling eccentricity and difficulty in including very high spins.

4.1.1. Radiation content. In the majority of current simulations, the initial data contains spurious radiation (also known as *junk* radiation) in the neighbourhood of the black holes, due to simplifications made when constructing the initial data (in particular the conformal-flatness assumption). It also does not contain the radiation which would have resulted from the evolution of the binary from early times. The spurious radiation is visible in BBH waveforms only at early times, and is followed by the astrophysically expected waveform. Typically the initial part of the waveform must be discarded, and the spurious radiation can also cause unphysical numerical reflections from mesh refinement or outer boundaries. In [131], the authors propose a new method of constructing initial data based on the PN approximation. This initial data set is not conformally flat, and contains the radiation expected from the previous inspiral. One drawback of this method is that the Einstein constraint equations are satisfied only to a given PN order. In [132], another type of initial data, also constructed using the PN method [133], is evolved. This initial data is also constructed to satisfy the constraint equations to a given PN order, as with previous approaches [134]. The resulting evolution gives the expected waveform from the start and contains significantly less spurious radiation than the evolution of comparable Bowen-York initial data. On the other hand, there is significantly higher orbital eccentricity ($e \sim 0.1$), as well as a variation in apparent horizon mass, perhaps caused by the constraint-violating nature of the initial data.

4.1.2. Eccentricity. Recently, in [135], a PN method was used for constructing low eccentricity initial data parameters, incorporating an EOB or Taylor Hamiltonian with Padé or Taylor expanded flux. This method was compared with previous PN methods [20, 136] and eccentricities comparable to those in [136] are obtained for equal-mass, non-spinning systems. Additionally, low eccentricities are obtained for systems with unequal masses and spins for a small selection of spin configurations.

4.1.3. High spins. Both the Bowen–York and CTS initial data approaches have intrinsic limits on the spins of the black holes which evolve from the initial data. This issue has been

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addressed recently in [137], where a comprehensive overview of the problems of high spin initial data is also presented. Whilst the dimensionless spins of the black holes on the initial data slice for Bowen–York and CTS initial data are found to be 0.9837 and 0.99 respectively, this spin quickly relaxes to about 0.93 after a short period of time (see also [60] where this was previously found for the Bowen–York case). A third type of initial data is considered, based on superposed Kerr–Schild solutions (with constraint solution), and this is shown to allow relaxed spins of above 0.99. Note that a modification to the standard puncture approach for head-on collisions can be used to produce high-spin puncture data as well [138, 139], and for the single black hole case [140], though this has not yet been studied for the orbiting case.

4.1.4. Constraint solution. When setting up a configuration of black holes for numerical simulation with Bowen–York initial data, it is necessary to solve the Einstein constraint equations, which are elliptic equations on the initial data slice. This can be computationally expensive, and the most commonly used solver code for this, `TwoPunctures` [141], uses a bi-spherical coordinate system which is specifically adapted to the case of two black holes. To increase flexibility, for example to investigate the possibility of simulating more than two black holes (see [142] for an alternative approach), in [143] an approximate analytic method was used to solve the constraint equations, based on [144]. It was found that the main effect of this approximation was to alter the eccentricity of the resulting evolutions, and when only the merger and ringdown are in-band, the mismatch between the waveforms with the exact and approximate constraint solution schemes was $<10^{-2}$.

4.1.5. Modifications to puncture initial data. Several studies of the properties of commonly used initial data have recently been performed. In [145], the propagation of modes in the puncture geometry is studied with spherically symmetric BSSN evolutions, and it is found that a potentially problematic numerical reflection of perturbations in the geometry does not occur due to a decoupling of the modes of the system. When initial data is constructed in the puncture technique, the coordinate conditions used in the evolution cause the geometry to change during the very first portion of the evolution and settle to the so-called *trumpet* solution. In both [146] and [147], initial data is constructed which is already in the trumpet form. However, no significant difference is found in [146] between the evolution of trumpet and standard puncture data. In current BBH simulations, the evolution is usually performed on spatial slices which reach to spatial infinity. However, gravitational radiation is properly defined only at future null infinity (see the discussion in section 4.3). An alternative is to construct slices which asymptote to null infinity rather than spatial infinity, and one way to do this is to use *hyperboloidal* slices. In [148], Bowen–York initial data including unequal masses, spins and boosts is generalized to such hyperboloidal slices. The evolution of this initial data should allow extraction of gravitational radiation at future null infinity, removing a common source of error in BBH simulations.

4.2. Boundary conditions

Typical NR BBH simulations begin with a three-dimensional initial data set and evolve this forward in time. Due to the difficulties of simulating an infinite spatial domain with finite numerical resources, a finite domain is usually simulated in combination with an artificial boundary condition on the exterior of the domain. Ideally, these boundary conditions should result in a solution which is indistinguishable from an evolution with an infinite spatial domain. This can only be achieved approximately, and the boundary conditions should have certain properties to give a useful solution. Firstly, they should not contaminate the solution with

unphysical gravitational radiation, either due to reflections of the waves generated by the binary, or due to radiation generated by the boundary condition itself. Secondly, they should be *constraint preserving* to yield a result which is a solution to the Einstein equations. Thirdly, they should result in a *well-posed initial boundary value problem*. This is a mathematical property which is a necessary condition for the numerical schemes used to be formally stable. These three properties are often only approximately satisfied, but the effects can be included in estimated error bars on the physical results of the simulation.

Current evolutions using the SpEC code in the generalized harmonic formulation such as those in [39, 40] use an outer boundary condition designed to satisfy the Einstein constraint equations as well as to minimize the incoming gravitational radiation [31, 149, 150], though these are not designed to be mathematically well posed (a necessary condition for formal stability of the problem under small perturbations). Recently, in [151], boundary conditions for the generalized harmonic formulation have been presented which are constraint-preserving and of the Sommerfeld type, which limits reflections of waves off the boundary. Additionally, the initial boundary value problem is well posed.

BSSN simulations generally apply an outgoing radiative boundary condition by modelling the solution at the boundary as a radially propagating outgoing wave [152]. This approach is designed to reduce reflections of the outgoing radiation into the numerical grid which would contaminate the solution. However, it is neither mathematically well posed nor does it respect the Einstein constraint equations. It is expected that the errors introduced are smaller than the errors due to finite differencing, but this has not been comprehensively studied for long simulations. One approach is to place the outer boundary sufficiently far from the binary that the waveforms measured at finite radius are out of causal contact with the outer boundary, and this was the approach taken in the early short simulations as well as in modern simulations for which this is sufficiently inexpensive (for example those in [153]). In [154], new boundary conditions for the BSSN evolution system are proposed which exactly satisfy the constraint equations, specify approximately zero incoming radiation and are stable (the initial boundary value problem is well posed) to a linear order. It is hoped that these boundary conditions can be used in evolutions in future to avoid the above-mentioned problems.

4.3. Gravitational-wave extraction

Mathematically, gravitational radiation from a BBH inspiral and merger is defined at future null infinity, i.e. the part of the spacetime towards which all null rays, such as light or GWs, propagate. Current NR BBH codes are based on a Cauchy, 3+1, formalism, which means that initial data is specified on a (portion of a) three-dimensional spacelike slice and then evolved forwards in time. This leads to a sequence of spacelike slices on which the solution is known. GWs must be read off at a finite spatial radius, and this introduces an error in the waveform. An obvious solution is to compute the radiation at several radii and extrapolate the waveform to infinite radius as a function of retarded time from the source. It was shown in [155] that this is not a trivial procedure, and a detailed analysis and successful extrapolation of the inspiral portion was presented in [39]. A failure to extrapolate waveforms from the SpEC code can lead to a phase error of 0.5 radians [39], or a mismatch of $\sim 10^{-2}$ [156], if using waveforms extracted at $r = 50M$ only.

A detailed study of two different techniques for performing this extrapolation is reported in [156]. The first method involves extrapolating the amplitude and phase of the complex waveform at each instant of time using various orders of polynomial extrapolation. Essentially, this is the technique which is now common in the literature, though in [156] various refinements are proposed which are shown to improve the quality of the extrapolation. The second

method, based on ideas in [155], involves expressing the amplitude and time as a function of the phase and then performing the extrapolation. Error estimates are made, and the two methods are shown to agree within these error estimates. However, there were problems with the convergence of both methods after the merger which were not properly understood, and future work will investigate these. This study applies only to the waveforms from the SpEC code, and the same conclusions might not hold for waveforms produced by other codes. Generally, numerical relativists have found that it is necessary to be extremely careful with the extrapolation procedure, and, as pointed out in [156], there are still issues to be resolved.

In [157], wave extraction techniques at finite radius are studied and it is shown that the conventional extrapolation of waveforms extracted at low radii is consistent with extracting at $r = 1000M$. The use of such a large extraction radius is possible because of the constant angular resolution in the NR evolution code, as demonstrated for a lower extraction radius in [39, 62]. The outer boundary can be placed out of causal contact with the wave extraction sphere without incurring inordinate computational cost. The peeling property of the Weyl scalars is also studied, and while ψ_4, ψ_3 and ψ_2 decay with distance from the source with the expected exponent, the situation for ψ_0 and ψ_1 is more complicated, and different exponents are obtained. One suggested explanation for the differing exponents is coordinate and frame effects in the wave extraction procedure, but it is also pointed out that the peeling property might not be expected to hold even for single spinning Bowen–York black hole spacetimes, and by assumption it would not then hold for binaries either.

Instead of performing a traditional Cauchy evolution, where the solution is evolved along timelike directions, it is possible to evolve along null directions. This is called *characteristic* evolution. This cannot be done straightforwardly in the neighbourhood of the black holes as it leads to caustics in the solution, but it can be done in regions sufficiently far from them. The Cauchy- characteristic extraction (CCE) method combines the two approaches. Metric data is read at a sufficiently large radius from the solution generated by a Cauchy code and is used as input data for a characteristic evolution. In this way, the waveform can be evolved all the way to future null infinity, removing ambiguities due to coordinate conditions or insufficient distance from the source. This has been implemented in [158, 159] and represents the first unambiguous determination of GWs at future null infinity for a NR BBH simulation. Note that the outer boundary condition of the Cauchy evolution can still contaminate the waveform, but in this work the outer boundaries were causally disconnected from the CCE extraction worldtube, avoiding this problem. It was found that the waveform agreed with the extrapolated finite-radius waves within 0.2% in amplitude and within 0.01 radians in phase. It was also determined that the difference between extrapolated and CCE waveforms was not significant for GW detection, but that for Advanced LIGO, Advanced VIRGO and LISA, these differences might be important for parameter estimation.

4.4. Numerical methods

For numerical relativity evolution purposes, the four-dimensional BBH spacetime is usually foliated with three-dimensional spacelike slices. Each of these slices can be split into two regions with very different computational requirements. The region around the black holes has a complicated geometry reflecting the shapes of the horizons, but the region far from the black holes consists only of gravitational radiation. Since the radiation propagates essentially radially, it requires a constant angular resolution to resolve it. The majority of BBH NR codes today use Cartesian-type coordinates everywhere in the grid. These have the advantage of simplicity, as only a single coordinate patch is required to cover the entire simulation domain.

However, they are not efficient, as they lead to an increasing angular resolution with radius. If box-in-box mesh refinement is employed, this inefficiency can be partially addressed, but only at the expense of significantly reduced radial resolution.

In [160], multiple locally Cartesian coordinate patches adapted to the black holes and exterior spacetime were used with finite differencing methods and generalized harmonic evolution equations to compute an equal-mass, non-spinning BBH inspiral using excision techniques. The scalability and convergence were good, though the simulation developed instabilities before the merger. In [153], a similar patch structure was used for the exterior spacetime, but adaptive mesh refinement (AMR) with Cartesian grids was used for the region surrounding the black holes. The entire inspiral, merger and ringdown were simulated. In both these works, the fact that the exterior spacetime is resolved using constant angular resolution means that the computational cost in this region scales linearly with the radius. This means that the outer boundary of the domain can be placed out of causal contact with the region of physical interest for only moderate computational cost. This bypasses the problem that the correct outer boundary conditions for the BSSN formulation for the BBH problem are not known.

While most NR codes use finite differencing methods with global Cartesian coordinates, the SpEC code uses multiple coordinate patches as well as spectral methods. For simple equations, these methods can be shown to be significantly more accurate (exponential rather than polynomial convergence) for a given computational cost, and indeed, the quoted accuracy and efficiency on the waveforms from the SpEC code is impressive. In [47], a new gauge condition is presented along with a new grid structure (touching grids with penalty boundary conditions, rather than the previously used overlapping grids), as well as a new method of dynamically adapting the grids to the shapes of the black holes. With these new techniques, SpEC is able to handle a variety of configurations without fine-tuning the simulation parameters on a case-by-case basis during the merger phase as was previously required. Simulations of mass ratios of $q = 2$ and dimensionless spins of 0.4 are presented.

5. Challenges and conclusions

In this work, I have given a brief overview of the current state of BBH simulations in NR. It is now possible to simulate BBH systems over periods as long as 15 orbits for low mass ratios and moderate spins, or to simulate a smaller number of orbits for mass ratios up to 1:10 or dimensionless spins up to 0.92. Pushing these simulations to higher numbers of orbits, mass ratios and spins can be achieved but at significant computational cost. For arbitrary spin configurations, it is not known how many black hole orbits are needed from NR before a sufficiently accurate complete waveform using input from analytic methods can be constructed. In order to span the parameter space of initial spins and mass ratios, many simulations will be needed. These are still very expensive to perform, taking weeks or months on up to a thousand CPUs for high mass ratios and large numbers of orbits.

Approximately speaking, the computational cost of a BBH simulation scales with the mass ratio q, based on the resolution requirement of the smaller black hole alone. For an accurate equal-mass, non-spinning eight orbit simulation which takes on the order of 200 000 CPU hours, a simple estimate shows that scaling this to a mass ratio of $q = 10$ would take 2 million CPU hours, and this is probably an underestimate, as the fact that the waveform gets longer with increasing q has not been considered, nor the fact that the higher resolution required around the smaller hole will not always come with perfect computational scaling. Since many simulations for different spin configurations would be required to construct or tune template banks used in GW data analysis for detection and parameter estimation, this is

clearly infeasible (computer resources for NR BBH groups for an entire year are usually of the order of a few million CPU hours).

There are also theoretical issues which need to be better understood. As explored in [156], the extrapolation of finite radius waveforms is not yet perfect, especially in the neighbourhood of the merger. Cauchy-characteristic extraction for BBH systems [158, 159] should in principle solve this problem, but its use is not yet widespread. It is also not yet clear exactly how to construct accurate waveforms from PN and NR results when the PN waveforms come with their own intrinsic errors. It has been shown [76] that most of the different PN approximants can be used equally well for detection with ground-based detectors of systems below a certain total mass (12 $M_\odot$), indicating that the errors in each of these approximations are not significant for the low frequencies for which such systems are in-band. However, for higher masses, and for parameter estimation, the PN errors become significant, and assuming that they are zero when constructing PN–NR waveforms is not necessarily the best choice.

The generation of the gravitational recoil around the BBH merger is not understood in precise terms. Simple analytic models have been tested [53, 91, 94, 95] and shown to fit well with numerical data. However, the models are *a posteriori* empirical fits to forms qualitatively inspired by PN predictions in a region where the agreement with PN is poor. Also, the crucial identification of the orbital plane is gauge dependent. To get a robust, coordinate-independent understanding of this recoil will require detailed understanding of the physics in the region near the black holes. The work of Lovelace *et al* [107], where the linear momentum in this region is computed, may be a starting point for this. The previous work [161] has also analysed the features of the recoil, showing that a Newtonian model containing some input from the simulations combined with a Kerr quasi-normal mode expansion is able to reproduce the numerical results. There has also been recent work [162, 163] combining PN with perturbation theory in the close-limit approximation [164] where the recoil for non-spinning black holes is computed and agrees moderately well with NR results. The extension of this work to black holes with spins should lead to a greater insight into the generation of the recoil.

There have been recent theoretical advances which are not yet routinely incorporated in numerical simulations. More astrophysically realistic initial data prescriptions have been given [131, 133], and initial evolutions performed [132]. It is not clear to what extent the constraint violations present in these initial data sets will impact their usefulness, and this needs to be studied further. A method for constructing initial data for almost maximally spinning black holes has also been proposed [137] which goes beyond the capabilities of the Bowen–York initial data currently used by many groups. Two possibilities for improving the physical accuracy of gravitational waveforms from BBH simulations have recently been explored: hyperboloidal slicing conditions [148], in which future null infinity is approached in the computational domain, and Cauchy-characteristic extraction [158, 159], where the waveforms are evolved to future null infinity using a separate null code. Whilst it is shown that the CCE waveforms are consistent with currently used extrapolation techniques, this picture may change as simulations become more accurate.

In summary, there are many interesting problems to be addressed in vacuum NR. In terms of physics, these include gaining improved understanding of the strong field geometry around the black holes, and how this affects the final black hole produced in the merger. Computationally, increased efficiency for long inspirals, very high spins, and higher mass ratios are the main challenges. Finally, a strong interaction with the community of GW data analysts will be necessary to fully leverage the exciting progress that has been made in NR to date.

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