THE FINAL STATE FROM GENERIC BINARY BLACK HOLE COALESCENCE: MASS, SPIN, AND GRAVITATIONAL RECOIL

A Dissertation in
Physics
by
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Submitted in Partial Fulfillment
of the Requirements
for the Degree of

Doctor of Philosophy

December 2009
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Abstract

Since the breakthroughs of numerically solving Einstein’s Equations of gravity in the early 21st century, numerical relativity has been used primarily to study the most astrophysically relevant binary black hole configuration, the quasi-circular inspiral. Various aspects of the quasi-circular system with different spin configurations have been studied, including the gravitational radiation and the final state of the spacetime, that is, its mass, spin, and recoil velocity (or kick). However, these quasi-circular configurations cover a small sliver of the parameter space of solutions for binary black hole spacetimes. This dissertation explores the final state from generic binary black hole coalescence, considering a broad range of initial orbital configurations, from direct plunges to escape and recapture events to quasi-circular inspirals and to even more energetic orbits.

Gravitational recoil is caused by the anisotropic emission of gravitational radiation due to asymmetries in the initial binary black hole spacetime. For quasi-circular inspirals, the beamed radiation tends to average over the inspiral, with the main contribution coming from the plunge. By considering hyperbolic encounters that are plunge-dominated, we observe an enhancement of the preferential beaming leading to kick velocities of $\sim 10,000$ km s$^{-1}$ for the sequence studied, about $2.5 \times$ larger than the highest projected kick from a quasi-circular configuration. Despite the higher magnitude kicks produced, these systems exhibit the same general dependence of the kick on the initial spin configurations as the quasi-circular system.

The final spin of the system is determined by the residual orbital and spin angular momentum that is not radiated in the process of merging. Considering plunge-dominated systems with a broad range of initial spin configurations and impact angles provides a comprehensive search of those configurations that maximize the final spin of the remnant black hole. We estimate that the final spin can reach a maximum $a/M_h \approx 0.992$ for extremal spinning, equal-mass black hole mergers. In addition, we find that as one increases the orbital angular momentum, the mergers produce black holes with mass and spin oscillating around the values of a golden black hole. We find that the values of the parameters for the golden black hole correspond to the final state of the black hole obtained from the quasi-circular system with the same spin configuration. Lastly, we confirm that zoom-whirl behavior can survive the dissipatory drain of full General Relativity and is not confined to a finely tuned region of initial parameters.
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List of Symbols

Conventions defined in Section A.

\( g_{\mu\nu} \) Four-dimensional spacetime metric, p. 5
\( \gamma_{ij} \) Three dimensional spacetime metric, p. 6
\( \tilde{\gamma}_{ij} \) Conformal spatial metric, p. 10
\( R_{\alpha\beta\mu\nu} \) Riemann curvature tensor, p. 6
\( R_{\mu\nu} \) Ricci tensor, p. 5
\( R \) Ricci scalar, p. 5
\( (3) R_{\alpha\beta\mu\nu} \) Spatial projection of the Riemann curvature tensor onto \( \Sigma \), p. 7
\( (3) R \) Spatial Ricci scalar, p. 8
\( \tilde{R}_{ij} \) Conformal Ricci tensor, p. 12
\( \tilde{R}_{ij}^{\phi} \) Conformal part of the Ricci tensor related to \( \phi \), p. 12
\( T_{\mu\nu} \) Stress Energy tensor, p. 5
\( \rho \) Energy density measured by observer \( n^\mu \), p. 8
\( j_\mu \) Momentum density measured by observer \( n^\mu \), p. 8
\( S_{ij} \) Spatial Stress Energy tensor, p. 8
\( S \) Trace of spatial Stress Energy tensor, p. 8
\( n^\mu \) Timelike normal to the hypersurface \( \Sigma \), p. 6
\( \Sigma \) Three-dimensional Cauchy hypersurface foliated by \( n^\mu \), p. 6
\( P^\alpha_\beta \) Projection operator of four-dimensional quantities onto \( \Sigma \), p. 6
$K_{ij}$  Spatial extrinsic curvature, p. 6
$K$  Trace of the extrinsic curvature, p. 8
$A_{ij}$  Traceless extrinsic curvature, p. 10
$\tilde{A}_{ij}$  Conformal traceless extrinsic curvature, p. 11
$\nabla_\alpha$  Covariant derivative compatible with $g_{\mu\nu}$, p. 6
$D_i$  Spatial projection of the covariant derivative onto $\Sigma$, compatible with $\gamma_{\mu\nu}$, p. 7
$\tilde{D}_i$  Covariant derivative associated with $\tilde{\gamma}_{ij}$, p. 11
$L_{\vec{n}}$  Lie derivative along $n^\mu$, p. 6
$\alpha$  Lapse, p. 7
$\beta^i$  Shift vector, p. 7
$\det g$  Determinant of $g_{\mu\nu}$, p. 9
$\mathcal{H}$  Hamiltonian constraint, p. 9
$\mathcal{M}_i$  Momentum constraint, p. 9
$\psi, \chi, \phi$  Different choices of conformal factors, p. 10
$\tilde{\Gamma}^i$  Conformal connection functions, p. 11
$P^i$  Bowen-York extrinsic curvature momentum parameter, p. 14
$S^i$  Bowen-York extrinsic curvature spin parameter, p. 14
$m_{(c), \pm}$  Puncture bare masses, p. 14
$M_{adm}$  ADM mass of the spacetime, p. 15
$M_{irr}$  Irreducible mass, p. 22
$M_\Delta$  Local mass of $S$, or the Christodoulou Mass, p. 24
$J_\Delta$  Local Angular Momentum of $S$, p. 23
$\Psi_4$  Fourth Weyl Scalar, p. 26
$C(t, r)$  Time and radial dependence of $\Psi_4$, p. 26
$-2Y_{lm}$  Spin weight -2 spherical harmonics, p. 26
$a^* M_h$  Golden spin value, p. 60

$\frac{M_h^*}{M}$  Golden mass value, p. 60

$q$  Amount of precession between apocentres, p. 75

$w$  Number of whirls per zoom, p. 75

$v$  Order in which zoom leaves are traced out, p. 75

$z$  Number of zooms, p. 75

$d/M$  Initial coordinate separation, p. 33

$r/M$  Coordinate separation, p. 34

$t/M$  Coordinate time, p. 34

$\phi/2\pi$  Orbital phase, p. 66

$\vec{P}/M$  Initial momentum of the BHs, p. 33

$L/M_{adm}^2$  Initial orbital angular momentum of the system, p. 44

$J/M_{adm}^2$  Initial angular momentum of the system, orbital plus spin, p. 51

$S/M^2$  Initial total spin of the two BHs, p. 51

$\theta$  Impact angle, the angle between the initial momentum and the vector connecting the two BHs, p. 51

$a/M_h$  Final spin of the remnant BH, p. 60

$M_h/M$  Final mass of the remnant BH, p. 60
Acknowledgments

First and foremost, I would like to thank my girlfriend of 10 years and now my wife, Allison, for all her support and friendship. I am truly thankful that she has stuck with me over this past decade. I would be lost without her.

There are several people that I have worked with over the past few years that I would also like to thank. I would like to thank my co-advisers, Pablo Laguna and Deirdre Shoemaker, who both endured a ‘long distance’ research arrangement with me for the past year and a half, and for introducing me to the field of numerical relativity. It has not been easy, but it certainly has been fun, and I look forward to and am excited to work with them in the future. Richard Matzner has also been of instrumental value to my research at Penn State and I am truly thankful for his help. There have been many ‘skype’ calls between Richard, Pablo, and myself, where truly brilliant ideas have been formulated. I also have had the privilege to work with Janna Levin of Columbia University on Zoom-whirl dynamics, and it was a pleasure.

I would also like to thank Ian Hinder, Frank Herrmann, Tanja Bode, and Roland Haas, for all their guidance and patience helping me learn the ins and outs of the MayaKranc code, as well as enlightening conversations about NR. I would also like to thank them, Eloisa Bentivegna, Erik Schnetter, Marcus Ansorg, and Andrew Knapp, for their contributions to the MayaKranc code.

I have spent many afternoons discussing my research and other things with my great friend, Paul Van Noordt, of The University of Texas at Austin. I thank him for his encouragement and friendship.

Finally, I would like to thank my family, especially my Mom and Dad, my brother, Joey and his daughter, Olivia, my sister, Kim, and my niece Julia for always being there for me.

Work supported in this dissertation in part by NSF grants PHY-0653443, PHY-0555436, PHY-0653303, PHY-0114375, PHY-0354842, PHY-0914553, PHY-0855892, PHY-0925345 and NASA grant NNG-04GL37G. Computations were carried out under LRAC allocation MCA08X009 and at the Texas Advanced Computation Center, The University of Texas at Austin on clusters Lonestar and Ranger.
To my wife, Allison
Chapter 1

Introduction

Until the 20th century, our understanding of the universe was based almost entirely on human observation; that is, what could be seen with the naked eye. The advent of technologies able to detect electromagnetic radiation other than visible light allows the universe to be studied in a completely new manner. Another spectrum of radiation that is just now on the cusp of detection, gravitational radiation, promises to provide an additional avenue and new insight into the workings of the universe. This prospect of detection of gravitational waves has energized the entire field of numerical relativity (NR), which focuses on the numerical solution to Einstein’s Equations of gravitation. Compact binaries, for example, black hole (BH) or neutron star binaries, are considered some of the most likely sources of gravitational waves for detection by the ground-based Laser Interferometer Gravitational Wave Observatory (LIGO) [122] and the future space-based Laser Interferometer Space Antenna (LISA) [124]. Over the past decade, several gains have been made in evolving binary black hole (BBH) spacetimes numerically, and there is an abundance of BBH waveforms available for use with matched filtering techniques. Undoubtedly, these waveforms will be crucial to the first detection of gravitational radiation in the very near future.

Numerical relativity is the only method available to obtain a full gravitational waveform. Any quasi-circular BBH system has three stages. The first is the inspiral, where the BHs orbit each other in a near circular orbit, slowly approaching as radiation is emitted. The second stage is the plunge and merger, in which the BHs quickly fall in and merge into a single distorted BH, called the remnant. The final stage is the ringdown, where the distorted BH continues to radiate until a stationary state is reached, generally a Kerr BH [106, 107]. The inspiral waveform can be accurately generated via post-Newtonian (PN) approximations, and the ringdown can be modelled as the super-
position of quasi-normal modes. However, the plunge and merger waveforms can only be obtained through a full NR simulation. Further, a full simulation is critical to compare the final parameters (mass, spin, kick) of the spacetime to its initial configuration, which is the majority of the work presented in this dissertation.

BBH systems are also important for another reason. General Relativity works extremely well in the weak-gravity limit, explaining the precession of Mercury’s perihelion, and predicting the bending of light around massive objects like the Sun. However, there have been no strong field tests yet for General Relativity, and numerical relativity and the gravitational radiation generated by BBH spacetimes could unveil evidence supporting GR in this strong field regime, or possibly indicate that an alternative theory of gravity should be considered.

We are at a very exciting period in scientific history, with the ability to detect gravitational waves on the horizon, and the possibility of gaining more support for Einstein’s elegant theory of gravitation. Without developments in the evolution of BBH spacetimes in NR and the revolution in computer processing, the detection of gravitational waves would not be within grasp. In the next sections, I review the history of BBH simulations and give motivation for the work presented in this dissertation.

1.1 History of Binary Black Hole Simulations

The numerical study of BBH spacetimes has progressed greatly since the first study of two “wormholes” by Hahn and Lindquist in 1964 [90] and the the first extraction of primitive gravitational waveforms by Smarr [159] and Eppley [77] in the head-on collision of two BHs in 1975. The field lay dormant until the advent of LIGO in the early 1990s, with the possibility of actual gravitational wave detection and the need for a template bank of expected gravitational waves being the driving force of renewed interest. It was during this period that the field flourished with the development of the main components of accurate and stable evolutions of BBH spacetimes. During these years, the Arnowitt-Deser-Misner (ADM) 3+1 decomposition of spacetime was reformulated into the Baumgarte-Shapiro-Shibata-Nakamura (BSSN) equations, with much improved stability properties [25, 156]. Brandt and Brügmann developed a ‘puncture’ method for solving the initial data problem over the entire computational domain [41]. The computer revolution of the 1990s resulted in high-performance computers capable of handling the extensive computational resources needed for a full 3D BBH spacetime. There are some very good reviews of NR given by Baumgarte and Shapiro [26] and,
more recently, Alcubierre [3]. The combination of all these developments has allowed the field of numerical relativity to blossom in recent years.

There are two main formulations used for BBH spacetime evolutions: the first uses a BSSN formulation of Einstein’s Equation (used by the PSU-GATech group and discussed in detail in Chapter 2) and the second uses a formulation of Einstein’s Equations in generalized harmonic coordinates [140, 141, 142]. Both formulations have led to breakthroughs in NR. In 2003, one full orbital period was simulated by Brügmann et al. [45] and in 2005, three independent groups evolved a full BBH spacetime, from inspiral through merger and ringdown, and for the first time, extracted gravitational radiation from the merger phase [17, 53, 140]. The majority of the physics from BBH simulations has been accumulated within the past four years. The field quickly transitioned to the study of the gravitational recoil (or kick) of the remnant BH due to the asymmetric beaming of gravitational radiation during the plunge. Kicks from both unequal-mass, non-spinning systems [18, 84, 85, 97] and spinning systems were studied [62, 98, 99, 126, 139, 154, 165], with one very interesting result of kick velocities up to $\sim 4000 \text{ km s}^{-1}$ [59] obtained. The highest kick simulated prior to this dissertation was $\sim 3300 \text{ km s}^{-1}$ [65]. This discovery sparked much excitement in the astrophysics community, since velocities of that magnitude could eject a Super-Massive Black Hole (SMBH) from the core of a galaxy. Great effort has gone into understanding the dependence of these “superkicks” on the mass ratio [13, 127] and analytic formulas have been developed based on the NR results [58]. The final parameters of the remnant BH (mass, spin) for quasi-circular orbits have been studied [16, 54, 128, 147] and analytic fits and models for the final spin have been developed [39, 40, 47, 145, 146, 166]. The circularization of BBH systems with non-zero initial eccentricity [100, 101, 161] has also been a topic of study.

Gravitational radiation has been the staple of these BBH systems thus far, with many aforementioned references presenting the radiation from inspiral, merger, and ringdown. In addition, there have been studies done focused on primarily the gravitational waveforms: from the last circular orbit [56], comparison of waveforms generated by different code formulations [15], and using the waveforms to calculate radiated quantities [14]. Many of these waveforms were used in the Numerical INJection Analysis (NINJA) project to test the sensitivity of current data analysis techniques, including matched filtering [10, 49]. Techniques for comparing and stitching post-Newtonian waveforms and NR waveforms have been developed [2, 19, 20, 91]. Matched filtering techniques [67] have been used to compare NR waveforms at different resolutions and spin configurations [158, 168], as well as waveforms generated with different initial data [34]. With the
aid of NR waveforms and Advanced LIGO reaching design sensitivity, the first detection of gravitational radiation may occur very soon.

1.2 Motivation

With the most astrophysically relevant BBH configuration (quasi-circular) extensively studied, many NR groups have shifted their focus to the study of non-vacuum numerical systems. However, there is still physics left to be uncovered for vacuum systems, since quasi-circular configurations cover only a very small sliver of the parameter space of BBH systems. The research presented in this dissertation is concerned with these unexplored regions of parameter space, with focus on the final mass, spin, and kick of the remnant from generic BBH mergers. Finding the answers to the following interesting questions has been the motivation of this research: Since the main contribution to the kick velocity is from the plunge of the BHs, how do plunge-dominated systems affect the final kick? Can an extremal spin BH \((a/m = 1)\) be obtained from the merger of two BHs? Even more intriguing, is the cosmological censorship conjecture broken \((a/m > 1)\) for any merger of two BHs? Do the orbits of the BHs exhibit zoom-whirl behavior? If so, are the waveforms distinct from the quasi-circular waveforms? What happens to the final mass and spin of the remnant as initial angular momentum is increased and for different impact parameters? To answer these questions, we will use NR as a tool for discovery to probe the final state from generic BBH coalescence.

In Chapter 2, I discuss the background theory for the 3+1 decomposition of spacetime and the Moving Puncture Recipe (MPR) and how they are implemented computationally. The calculations of mass, spin, and kick of a BH are discussed in Chapter 3. Chapter 4 discusses the results of plunge-dominated mergers on the final kick of the BH, producing the largest simulated kick velocity to date. Chapter 5 presents the results of the most extensive study of the parameter space of BBH spacetimes. From this study, we are able to make a prediction for the largest possible spin attainable from equal-mass BBH mergers and observe intriguing oscillations in the final mass and spin parameters. Chapter 6 presents an introduction to zoom-whirl orbits, their common place in BBH spacetimes, and the distinct gravitational waveforms produced from these highly precessing orbits. Finally, Chapter 7 summarizes the results of the previous chapters, and concludes with a look towards the future. The notation and conventions adopted for this dissertation can be found in Appendix A.
Chapter 2

Numerical Relativity: Theory and Infrastructure

Numerical relativity deals with the numerical solution of Einstein’s Field Equations (EFE):

\[ G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R = 8\pi T_{\mu\nu}, \]  \hspace{1cm} (2.1)

where \( R_{\mu\nu} \) and \( R \) are the Ricci tensor and scalar respectively, \( g_{\mu\nu} \) is the four-dimensional spacetime metric, and \( T_{\mu\nu} \) is the stress-energy tensor. The beauty of the EFE is that they are written in a purely covariant way, with no distinction between ‘space’ or ‘time’, but a unification of the two, ‘spacetime’, where each is treated with an equal footing. However, this unification is one of the main roadblocks in being able to numerically solve the EFE effectively. This is because numerical techniques are formulated for the use with Initial Value Problems (IVPs), or Cauchy Problems, where initial data is specified and then evolved in time using evolution equations. Therefore, a reformulation of the EFE to give a sense of a ‘time’ direction is desired. Further, solving the EFE numerically is a daunting, non-trivial task. The EFE consist of a set of ten coupled, second-order partial differential equations for the spacetime metric, \( g_{\mu\nu} \). Since \( \nabla^\mu G_{\mu\nu} = 0 \), not all ten equations are independent of each other, but there are constraint equations that must be solved in addition to the evolution equations. In other words, the initial data cannot be specified freely, but must satisfy these constraint equations, otherwise the solution found is not one of the EFE. Further, the correct choice of gauge (or coordinates) must be made, otherwise the evolution may become unstable due to the formation of coordinate singularities or other grid pathologies. In this chapter, I will address these issues, specifically discussing two 3+1 formulations of spacetime, the Arnowitt-Deser-
Misner (ADM) and Baumgarte-Shapiro-Shibata-Nakamura (BSSN) formulations for the evolution and constraint equations, Bowen-York extrinsic curvature and punctures for initial data, and the fiducial choice of gauge used throughout the numerical relativity community.

2.1 3+1 Foliation of Spacetime and the ADM Equations

There are several approaches setting the EFE into an IVP \([90, 140]\) but the one implemented by the PSU-GATech numerical relativity group and the one discussed in this section is the 3+1 Formulation of Spacetime, where 3+1 stands for three spatial and one time dimension. We start by foliating our four-dimensional spacetime manifold with metric, \(g_{\mu\nu}\), into three-dimensional Cauchy hypersurfaces, \(\Sigma\), by finding the timelike normal to \(\Sigma\), \(n^\mu\). This foliation induces a three-dimensional metric on \(\Sigma\), as

\[
\gamma_{\mu\nu} = g_{\mu\nu} + n_\mu n_\nu.
\]

Through \(\gamma_{\mu\nu}\), we can project four-dimensional quantities onto \(\Sigma\) with the projection operator,

\[
P^\alpha_\beta = \delta^\alpha_\beta + n^\alpha n_\beta,
\]
creating three-dimensional, purely spatial quantities on \(\Sigma\).

In addition to the manifold’s intrinsic curvature, defined through the Riemann curvature tensor, \(R_{\alpha\beta\mu\nu}\), we also need to know how the three-dimensional hypersurface, \(\Sigma\), is embedded in the four-dimensional manifold. This quantity is called the extrinsic curvature and can be defined as the parallel transport of the normal vector projected onto \(\Sigma\):

\[
K_{\mu\nu} := -P^\alpha_\mu \nabla_\alpha n_\nu = -(\nabla_\mu n_\nu + n_\mu n^\alpha \nabla_\alpha n_\nu).
\]

The extrinsic curvature can also be written as a Lie derivative along the normal vector of \(\gamma_{\mu\nu}\):

\[
K_{\mu\nu} = -\frac{1}{2} \mathcal{L}_{\bar{n}} \gamma_{\mu\nu}.
\]

Equation 2.5 writes the extrinsic curvature as a Lie derivative along the normal vector, and if the normal vector is in the direction of time, this would allow us to find \(\gamma_{\mu\nu}\) on hypersurfaces of different times. However, in general, the normal vector is not along the direction of constant spatial coordinates, since \(n^\mu \nabla_\mu t \neq 1\) but can be related...
to it by

$$t^\mu = \alpha n^\mu + \beta^\mu,$$

(2.6)

where $\alpha$ and $\beta^\mu$ are the lapse and shift, respectively. The time vector, $t^\mu$, relates the same coordinate points on one hypersurface to the next. Therefore, the lapse is an indication of how much proper time elapses between slices, and the shift indicates how the coordinates moved between slices. With this time vector, we can rewrite Equation 2.5 using properties of Lie derivatives to be in the direction of time:

$$\left( L_{\vec{t}} - L_{\vec{\beta}} \right) \gamma_{\mu\nu} = -2\alpha K_{\mu\nu},$$

(2.7)

where under further simplification and writing $L_{\vec{t}} = \partial_t$ we obtain

$$\partial_t \gamma_{\mu\nu} = -2\alpha K_{\mu\nu} + D_{\mu} \beta_{\nu} + D_{\nu} \beta_{\mu}.$$  

(2.8)

$D_{\mu}$ is the projection of the covariant derivative compatible with $g_{\mu\nu}$ onto $\Sigma$, that is $D_{\mu} = P^{\alpha}_{\mu} \nabla_{\alpha}$. Equation 2.8 is the first set of evolution equations of the ADM formulation and dictates how the spatial metric changes with time.

To find the remaining evolution equations and the constraint equations, projections onto the hypersurface and contractions with the normal vector of the Riemann curvature tensor are taken. Projecting all four indices of the Riemann tensor onto $\Sigma$ leads to the Gauss-Codazzi equation:

$$P^\delta_{\alpha} P^\xi_{\beta} P^\zeta_{\mu} R_{\delta\xi\zeta\lambda} = (3) R_{\alpha\beta\mu\nu} + K_{\alpha\mu} K_{\beta\nu} - K_{\beta\mu} K_{\alpha\nu},$$

(2.9)

where the superscript (3) denotes the Riemann tensor is the purely spatial curvature tensor on the hypersurface. Three projections and one contraction leads to the Codazzi-Mainardi equation:

$$P^\delta_{\mu} P^\zeta_{\alpha} P^\lambda_{\beta} n^\xi R_{\delta\zeta\lambda\xi} = D_{\mu} K_{\alpha\beta} - D_{\alpha} K_{\mu\beta}.$$  

(2.10)

From these equations, the Hamiltonian constraint, $\mathcal{H}$, and the Momentum constraint, $\mathcal{M}^\alpha$, can be derived (for full derivation see [170]). For brevity, I will just quote the results here, which come from using the Gauss-Codazzi equation for the Hamiltonian constraint, the Codazzi-Mainardi equation for the Momentum constraint, and projections and contractions of Einstein’s Equations (Equation 2.1). The Hamiltonian constraint and
Momentum constraint are

\begin{align}
(3) R + K^2 - K_{\mu\nu}K^{\mu\nu} &= 16\pi\rho, \quad (2.11) \\
D_\mu K^{\mu\alpha} - \mathcal{D}_\alpha K &= 8\pi j_\alpha, \quad (2.12)
\end{align}

where \( K = K^\alpha_\alpha \) is the trace of the extrinsic curvature and \( \rho = n^\mu n^\nu T_{\mu\nu} \) and \( j_\mu = -P^\nu_\mu n^\lambda T_{\nu\lambda} \) are the energy and momentum density measured by observer \( n^\mu \), respectively. These equations do not contain any time derivatives, and therefore must be satisfied independently on each spatial slice. Fortunately, if the constraints are satisfied initially, they will be satisfied on each successive hypersurface, guaranteed by the Bianchi Identities as shown by Fritelli [79]. Also note that the constraints do not depend on \( \alpha \) or \( \beta^\mu \). Therefore, they do not depend on our choice of coordinates but solely on the hypersurface.

Thus far, we have a system of evolution equations for the spatial metric, \( \gamma_{\mu\nu} \), and constraint equations that must be satisfied. The last piece of the ADM formulation is the evolution of the extrinsic curvature that can be found by taking projections and contractions of the Riemann tensor. Ricci’s equation can be found by two projections and two contractions of the Riemann:

\begin{equation}
P_\mu^\lambda P_\nu^\xi n^\delta n^\zeta R_{\delta\zeta\lambda\xi} = \mathcal{L}_n K_{\mu\nu} + \frac{1}{\alpha} D_\mu D_\nu \alpha + K^\lambda_\nu K_{\mu\lambda}. \quad (2.13)
\end{equation}

In this equation, we find a Lie derivative along the normal vector which we can relate to the time vector by Equation 2.6 to find an evolution equation for the extrinsic curvature. Again, for brevity, the details will be excluded, but through the use of the Gauss-Codazzi equation (2.9) and the EFE (2.1) the evolution equation for the extrinsic curvature is

\begin{equation}
\partial_t K_{\mu\nu} = \beta^\lambda \partial_\lambda K_{\mu\nu} + K_{\lambda\mu} \partial_\nu \beta^\lambda + K_{\lambda\nu} \partial_\mu \beta^\lambda - D_\mu D_\nu \alpha \\
+ \alpha \left[ (3) R_{\mu\nu} + K K_{\mu\nu} - 2K_{\mu\lambda} K^\lambda_\nu \right] + 4\pi\alpha [\gamma_{\mu\nu}(S - \rho) - 2S_{\mu\nu}], \quad (2.14)
\end{equation}

where \( S_{\mu\nu} \) is the projection of the stress-energy tensor onto \( \Sigma \), \( S_{\mu\nu} = P^\alpha_\mu P^\beta_\nu T_{\alpha\beta} \). Together with Equations 2.8, 2.11, and 2.12, these four tensorial equations comprise the ADM evolution equations. In the covariant form used thus far, it would seem that there are 20 evolution equations, with 5 constraint equations. However, we can choose a coordinate system that is well adapted to the 3+1 formulation in which only the spatial parts of three-dimensional spatial tensor will contribute. For example, since \( \gamma_{\mu\nu} \) is fully spatial, that is \( n^\alpha \gamma_{\alpha\beta} = n^\beta \gamma_{\alpha\beta} = 0 \), it has a reduced number of degree of freedoms
and we are free to only consider the spatial components, denoted as indices by Latin characters. Using this, we can specify the line element of our spacetime:

\[ ds^2 = g_{\mu\nu} dx^\mu dx^\nu = (-\alpha^2 + \beta_i \beta^i) dt^2 + 2\beta_i dt dx^i + \gamma_{ij} dx^i dx^j. \] (2.15)

We can also raise and lower purely spatial tensors with the spatial metric, \( \gamma_{ij} \). The determinant of \( g_{\mu\nu} \) is

\[ \sqrt{\det g} = \alpha \sqrt{\det \gamma}, \] (2.16)

where \( \det \gamma \) is the determinant of the spatial metric. In this coordinate system, the normal vector takes the form:

\[ n^\mu = (1/\alpha, -\beta^i/\alpha), \quad n_\mu = (-\alpha, 0). \] (2.17)

It is now clear that specifying the lapse and shift is equivalent to removing the coordinate degrees of freedom from the system. In addition, there are no evolution equations for the lapse or shift, and therefore they are freely specifiable (although it turns out that the choice of lapse and shift, or gauge choice, is central to stable simulations).

With the choice of coordinate system detailed above, the ADM equations can be rewritten in terms of purely spatial quantities. To summarize, the ADM equations are:

\[ \mathcal{H} = 0 = (3) R + K^2 - K_{ij} K^{ij} - 16\pi \rho, \] (2.18)

\[ \mathcal{M}_i = 0 = D_j K^j_i - D_i K - 8\pi j_i, \] (2.19)

\[ \partial_t \gamma_{ij} = -2\alpha K_{ij} + D_i \beta_j + D_j \beta_i, \] (2.20)

\[ \partial_t K_{ij} = \beta_k \partial_k K_{ij} + K_{ki} \partial_j \beta^k + K_{kj} \partial_i \beta^k - D_i D_j \alpha \]

\[ + \alpha \left[ (3) R_{ij} + KK_{ij} - 2K_{ik}K^k_j \right] + 4\pi \alpha [\gamma_{ij}(S - \rho) - 2S_{ij}]. \] (2.21)

The ADM equations as presented here are not in the original form as derived by Arnowitt, Deser, and Misner [7], which used a Hamiltonian formulation and the canonical momentum, \( \pi^{ij} \), instead of the extrinsic curvature, \( K^{ij} \), as the other dynamical variable (in addition to the spatial metric \( \gamma_{ij} \)). The reformulation using the extrinsic curvature was carried out by York [176].
2.2 BSSN Evolution Equations

Despite being the obvious choice of equations to use for numerical studies, in practicality the ADM equations are not stable enough for long running simulations. There are numerous reasons why. For one, the constraint violating modes do not propagate, but build up over the simulation leading to solutions that wander far off from solutions to Einstein’s Equations [4]. The ADM equations are not in a good mathematical form for numerical solutions as they are only weakly hyperbolic [3, Chapter 5, section 4]. Therefore, a reformulation of the ADM equations is needed that does not stray far from the constraint surface and that is hyperbolic in form. The first step is a conformal decomposition of the spatial metric and extrinsic curvature as pioneered by Nakamura, Oohara, and Kojima [132]. Further changes were implemented by Baumgarte and Shapiro [25], and Shibata and Nakamura [156] and therefore the reformulation is commonly known as the BSSN formulation of Einstein’s Equations. The new formulation was found to be vastly more stable than the ADM formulation in every spacetime studied [25]. In this section, I will discuss the BSSN formulation in use by the PSU-GATech Group. A full derivation of the BSSN equations can be found in [5].

There are four main differences between the BSSN and ADM formulations. First, the BSSN formulation includes a conformal rescaling of the spatial metric of the form

\[ \tilde{\gamma}_{ij} = \psi^{-4} \gamma_{ij}. \]  

The conformal factor, \( \psi \), is chosen such that the determinant of \( \tilde{\gamma}_{ij} \) is unity, that is

\[ \psi = (\det \gamma)^{1/12}. \]  

(2.23)

It turns out that \( \psi \) may not be the best variable to evolve, since it is not well behaved near the singularity. Therefore, there are different forms of conformal factors, related by

\[ \chi = \psi^{-4} = e^{-4\phi}. \]  

(2.24)

Both \( \chi \) and \( \phi \) are better behaved at the singularity. The PSU-GATech group evolves \( \chi \) as suggested by Campanelli et al. [53].

The next difference between the BSSN and ADM formulations is a decomposition of the extrinsic curvature into a traceless part, \( A^{ij} \), and its trace, \( K = K^i_i \):

\[ A_{ij} = K_{ij} - \frac{1}{3} \tilde{\gamma}_{ij} K. \]  

(2.25)
This decomposition is used because many slicing conditions (conditions for the lapse, see Section 2.3.3) are restrictions on $K$. As before, the traceless extrinsic curvature is conformally rescaled:

$$\tilde{A}_{ij} = \psi^{-4} A_{ij}. \quad (2.26)$$

In terms of $\chi$, the rescalings of $\gamma_{ij}$ and $A_{ij}$ are

$$\tilde{\gamma}_{ij} = \chi \gamma_{ij}, \quad \tilde{A}_{ij} = \chi A_{ij}. \quad (2.27)$$

The next addition is the introduction of auxiliary variables, known as the conformal connection functions, which are

$$\tilde{\Gamma}^i := \tilde{\gamma}^{jk} \tilde{\Gamma}_{jk} = -\partial_j \tilde{\gamma}^{ij}, \quad (2.29)$$

where $\tilde{\Gamma}_{jk}$ are the Christoffel symbols associated with $\tilde{\gamma}_{ij}$. These variables are promoted to dynamical variables and are evolved during the simulation. Therefore, there are 17 evolved variables, $(\chi, K, \tilde{\gamma}_{ij}, \tilde{A}_{ij}, \tilde{\Gamma}^i)$. There are also new constraints: the determinant of $\gamma_{ij}$ is 1, the trace of $A_{ij}$ is 0, and from the definition of the $\tilde{\Gamma}^i$ functions:

$$G^i = \tilde{\Gamma}^i - \tilde{\gamma}^{jk} \tilde{\Gamma}_{jk} = 0. \quad (2.30)$$

The introduction of the variables $\tilde{\Gamma}^i$ is of vital importance to the stable evolution of the system in that it allows for second derivatives of the conformal metric to simplify to either a scalar Laplace operator, $\tilde{\gamma}^{lm} \partial_l \partial_m \tilde{\gamma}^{ij}$, or to be replaced by spatial derivatives of $\tilde{\Gamma}^i$ [3].

The final change is the use of the constraints in the evolution equations for $\tilde{\Gamma}^i$ and $K$. Since the constraints are identically zero, there are an infinite number of ways that they can be added to the equations without changing the physical solution. However, the equations will be different mathematically, and the constraints can be added to put the equations into a stable form, yet keeping the same physical solution.

With these changes, the BSSN evolution equations become:

$$\partial_t \chi = -\frac{2}{3} \chi (\alpha K + \partial_j \beta^j) + \beta^i \partial_i \chi, \quad (2.31)$$

$$\partial_t \tilde{\gamma}_{ij} = -2\alpha \tilde{A}_{ij} + \beta^k \partial_k \tilde{\gamma}_{ij} \partial_j \beta^i - \frac{2}{3} \tilde{\gamma}_{ij} \partial_k \beta^k, \quad (2.32)$$

$$\partial_t K = -\chi (\tilde{D}^j \tilde{D}_j \alpha + 2\tilde{\gamma}^{ij} \partial_i \phi \cdot \tilde{D}_j \alpha) + \alpha (\tilde{A}_{ij} \tilde{A}_{ij} + \frac{1}{3} K^2 + 4\pi (\rho + S)) + \beta^i \partial_i K. \quad (2.33)$$
\[ \partial_t \tilde{A}_{ij} = \chi (\alpha \tilde{R}_{ij} + \alpha \tilde{R}^{\phi}_i - \tilde{D}_i \tilde{D}_j \alpha + 4 \partial_i (\phi \cdot \tilde{D}_j) \alpha - 8 \pi \alpha S_{ij} )^{TF} + \alpha \tilde{K} \tilde{A}_{ij} - 2 \alpha \tilde{A}_{ik} \tilde{A}^k_j \]
\[ + \beta^k \partial_k \tilde{A}_{ij} + 2 \tilde{A}_{j(i} \partial_j \beta^k - \frac{2}{3} \tilde{A}_{ij} \partial_k \beta^k, \tag{2.34} \]
\[ \partial_t \tilde{\Gamma}^i = \beta^j \partial_j \tilde{\Gamma}^i + \tilde{\gamma}^{jk} \partial_j \partial_k \beta^i + \frac{1}{3} \tilde{\gamma}_{ij} \partial_j \partial_k \beta^k - \tilde{\Gamma}^i_j \partial_j \beta^i + \frac{2}{3} \tilde{\Gamma}^i_j \partial_j \beta^j - \frac{4}{3} (\tilde{\Gamma}^i_j - \tilde{\gamma}^{kl} \tilde{\Gamma}^i_{kl}) \partial_j \beta^j \]
\[ - 2 \tilde{\gamma}^{ij} \partial_j \alpha + 2 \alpha (\tilde{\Gamma}^i_{jk} \tilde{A}^j_k + 6 \tilde{\gamma}^{ij} \partial_j \phi - \frac{2}{3} \tilde{D}^i K - 8 \pi \tilde{\gamma}^{ij} S_j), \tag{2.35} \]

where \( \tilde{D}_i \) and \( \tilde{R}_{ij} \) are the covariant derivative and Ricci tensor compatible with the conformal metric, \( \tilde{\gamma}_{ij} \), respectively. The Hamiltonian and Momentum constraints, Equations 2.18 and 2.19, become:

\[ \mathcal{H} = \chi \tilde{\gamma}^{ij} (\tilde{R}_{ij} + \tilde{R}^{\phi}) - \tilde{A}_{ij} \tilde{A}^{ij} + \frac{2}{3} K^2 - 16 \pi \rho, \tag{2.36} \]
\[ \mathcal{M}_i = 6 \tilde{A}^{ij} \partial_j \phi + \tilde{\gamma}^{jk} (\partial_k \tilde{\gamma}_{ij} - \tilde{\Gamma}^i_{jk} \tilde{A}_{il} - \tilde{\Gamma}^i_{ik} \tilde{A}_{jl}) - \frac{2}{3} \partial_i K - 8 \pi S_i. \tag{2.37} \]

The spatial Ricci tensor, \( (3) R_{ij} \), is related to the conformal Ricci tensor, \( \tilde{R}_{ij} \) by \( (3) R_{ij} = \tilde{R}_{ij} + \tilde{R}^{\phi}_{ij} \), where

\[ \tilde{R}^{\phi}_{ij} = -2 \tilde{D}_i \tilde{D}_j \phi - 2 \tilde{\gamma}_{ij} \tilde{D}^k \tilde{D}_k \phi + 4 \tilde{D}_i \phi \cdot \tilde{D}_j \phi - 4 \tilde{\gamma}_{ij} \tilde{D}^k \phi \cdot \tilde{D}_k \phi. \tag{2.38} \]

For numerical simulations, the BSSN formulation is much more stable than the ADM formulation for a variety of spacetimes. There may be a number of factors that contribute to this. The use of the constraints in the equations for \( K \) and \( \tilde{\Gamma}^i \) keep the system from diverging [81] and may put the system into a well-posed mathematical form with the property of hyperbolicity [28, 88, 89, 150]. Further, the constraint violations propagate at superluminal speeds, quickly leaving the computational domain [174]. This is in stark contrast to the ADM formulation, where the constraint violations do not propagate. Promoting the \( \tilde{\Gamma}^i \) to independent variables allows some of the less well-behaved terms to be rewritten in terms of \( \tilde{\Gamma}^i \) and its derivatives.

To code the BSSN equations by hand would be an incredibly time consuming and frustrating task. Fortunately, the BSSN equations are implemented using a Mathematica script called Kranc2BSSN that takes the equations in tensor notation and generates C code [104]. The code is arranged into a thorn for use by the Cactus infrastructure (see Section 2.4). The script generates the equations with different order stencils for the spatial derivatives, including second, fourth, and sixth order stencils. For most simulations presented in this dissertation, the sixth order stencil is used since it drastically reduces the accumulated error at the cost of the run speed of the simulation [102]. The exception
to this is the work presented in Chapter 4 and Section 5.1, which use fourth order stencils and were performed before the sixth order stencil was implemented. The gauge conditions are also generated by Kranc2BSSN (see Section 2.3.3). For time integration, a fourth order Runge-Kutta integrator and the Method of Lines are used.

2.3 Moving Puncture Recipe

Even with the stable 3+1 BSSN formulation, there are still two components needed: initial data for the first hypersurface and gauge conditions that avoid singularities and that can move the BHs throughout the computational domain. We achieve this through the Moving Puncture Recipe (MPR): Bowen-York extrinsic curvature and a puncture method to solve the Hamiltonian and Momentum constraints initially, and a modified gamma-freezing and 1 + log lapse for our gauge condition. Two of the three first successful full BBH simulations were accomplished in this way [16, 53].

2.3.1 Bowen-York Initial Data

Initial Data cannot be chosen freely for a spacetime, but must satisfy both the Hamiltonian and Momentum constraints, that is, Equations 2.18 and 2.19 in the ADM variables. In addition, we need a way to specify the BHs initial parameters (mass, spin, and momentum). To achieve this, we start by using a York–Lichnerowicz conformal transverse decomposition [121, 177, 178], where

\[
\gamma_{ij} = \psi^4 \tilde{\gamma}_{ij},
\]

\[
A^{ij} = K^{ij} - \frac{1}{3} \gamma_{ij} K,
\]

\[
\tilde{A}^{ij} = \psi^{10} A^{ij},
\]

where the bar is used to differentiate between this conformal decomposition and the one used in the BSSN formalism (Equations 2.22, 2.26), as used in [3]. Further, \( \tilde{A}^{ij} \) is decomposed into transverse and longitudinal parts. This allows us to solve the Momentum constraints under a few assumptions, and is known as the Bowen-York extrinsic curvature [37, 38]. The assumptions are that the extrinsic curvature is trace-free (\( K = 0 \)), conformal flatness (\( \tilde{\gamma}_{ij} = \eta_{ij} \)), and the BHs are in vacuum. The Momentum constraint then simplifies to

\[
D_j \tilde{A}^{ij} = 0,
\]
which has solution for $\bar{A}^{ij}$,

$$
\bar{A}^{ij} = \frac{3}{2r^2} \left[ P^i n^j + P^j n^i - (n^i n^j) P^k n_k \right] + \frac{3}{r^3} \left( \epsilon^{i k l} S_k n_l n^j + \epsilon^{j k l} S_k n_l n^i \right),
$$

(2.43)

where $P^i$ is the three-momentum of the black hole, $S^i$ is the spin, $\eta_{ij}$ is the flat spacetime three-metric, $n^i = x^i/r$, and $r = \sqrt{x^2 + y^2 + z^2}$. For multiple BHs, we can add multiple $\bar{A}^{ij}$'s for each individual BH together since the Momentum constraint, Equation 2.42, is linear. This amounts to

$$
\bar{A}^{ij} = \sum_{c=1}^{N} \bar{A}^{ij}_{(c)},
$$

(2.44)

where $N$ is the number of BHs in the spacetime. The extrinsic curvature is then

$$
K_{ij} = \psi^{-2} \bar{A}_{ij}.
$$

(2.45)

With this, the Momentum constraint is solved initially, and the Hamiltonian constraint (Equation 2.18) simplifies as well to

$$
\nabla^2 \psi = \frac{1}{8} \psi^{-7} A_{ij} A^{ij},
$$

(2.46)

where $\nabla^2$ is the flat Laplacian. We will not be as fortunate to have an analytic solution to the Hamiltonian constraint, and therefore need to solve it numerically. Cook achieved the first BBH initial data by solving Equation 2.46 with an isometry condition at the BH surface [64]. However, this method leads to the removal or excision of part of the computational grid in order to evolve the BH. There is another way in which we can solve the Hamiltonian constraint, the puncture method [41], which does not require excision.

### 2.3.2 Punctures

Previously, Equation 2.46 would be solved directly with the region around the BHs excised. This has two drawbacks: inner boundary isometry conditions where the excision occurred, and the necessity to locate the apparent horizon (AH) of the BH to know where to excise. The puncture method resolves both of these problems by positing the conformal factor, $\psi$, to have the form

$$
\psi = \frac{1}{a} + u,
\quad \frac{1}{a} = \sum_{c=1}^{N} \frac{m(c)}{2\left| \bar{r} - \bar{r}_{(c)} \right|},
$$

(2.47)
where \( m_{(c)} \) are the puncture masses, \(|\vec{r} - \vec{r}_{(c)}|\) are the coordinate distances to the punctures, and \( u \) is the regular part of the conformal factor. Inserting \( \psi \) into the Hamiltonian constraint, Equation 2.46, and using the fact that \( 1/a \) is a solution to the flat Laplacian in \( \mathbb{R}^3 \) with the points \( \vec{r}_{(c)} \) removed, the Hamiltonian constraint becomes

\[
\nabla^2 u + b(1 + au)^{-7} = 0, \quad (2.48)
\]

\[
b = \frac{1}{8} a^7 \tilde{A}^{ij} \tilde{A}_{ij}. \quad (2.49)
\]

The choice of the name punctures is now clear. Equation 2.48 is regular everywhere, since, at most, \( \tilde{A}^{ij} \tilde{A}_{ij} \) is proportional to \( 1/r^6 \) (Equation 2.43 with spin terms) and \( a \) is proportional to \( r \), where for simplicity \( r = |\vec{r} - \vec{r}_{(c)}| \). Then, as \( \vec{r} \to \vec{r}_{(c)} \), \( b \to 0 \) and the Hamiltonian constraint becomes \( \nabla^2 u = 0 \). Thus, the Hamiltonian constraint can be solved everywhere throughout the computational domain. Excision is no longer required and therefore neither are complicated inner boundary conditions or the necessity to locate the AHs (although we will find the AHs to calculate the mass and spin of the BHs, see Section 3.1). The ADM energy of the system can also be easily found for the initial data and is given by

\[
M_{adm} = \frac{1}{2\pi} \int b(1 + au)^{-7} d^3 x + \sum_{c=1}^{N} m_{(c)}. \quad (2.50)
\]

\( M_{adm} \) is assumed to be constant throughout the simulation and will be used in the global calculation of energy of the final BH (see Section 3.2).

The algorithm to initiate BBH spacetimes using Bowen-York initial data is as follows. The Momentum constraint is solved using the Bowen-York extrinsic curvature, Equation 2.43, by specifying the initial separation, \( d \), the initial momenta, \( P^i_{(c)} \), and the initial spins, \( S^i_{(c)} \), where \( c = 1, 2 \). Then, the spectral solver TwoPunctures [6] solves the elliptical Hamilton constraint equation, Equation 2.46. In order to normalize our spacetime to have unit total horizon mass, that is \( M_{h,1} + M_{h,2} = 1 \), TwoPunctures is used iteratively with a binary search algorithm to find the parameters \( m_{(1)} \) and \( m_{(2)} \). The ADM energy, Equation 2.50, is also calculated at this time.

Another interesting point about the initial data is due to the fact that we assume conformal flatness for a Kerr spacetime. It has been shown by Garat and Price that there is no solution for a Kerr BH that is both axisymmetric and conformally flat [80]. Therefore, we should not expect to obtain a Kerr BH alone with this initial data, and indeed we do not. However, we do obtain a Kerr BH with some extra spurious gravi-
tational radiation. The same phenomenon occurs for non-spinning BH spacetimes with some initial linear momentum; the solution is a boosted Schwarzschild BH plus some spurious radiation. This radiation is unphysical, and therefore we need to be careful with how it is dealt with when making physical measurements using the gravitational wave content of the system.

### 2.3.3 Gauge Conditions

The final piece of the MPR is the choice of gauge: to determine how the coordinates evolve from time step to time step. The gauge choice is equivalent to specifying equations for the lapse, $\alpha$, and the shift, $\beta^i$, and expends the coordinate freedom of Einstein’s Field Equations. The lapse and shift govern how much proper time passes and how the coordinates move between time slices, respectively. The gauge choice is crucial to stable evolutions and much fine-tuning [44, 169] has occurred since the first full numerical relativity simulations.

For the slicing condition, or the condition on the lapse, we use a modified Bona-Masso [5, 36] slicing condition of the form

$$\partial_0 \alpha = -\alpha^2 f(\alpha) K,$$

(2.51)

with $f(\alpha) = 2/\alpha$ and $\partial_0 = \partial_t - \beta^i \partial_i$. This is the so called ‘1+log’ slicing condition because, with zero shift, there is an analytic solution to the equation of the form

$$\alpha = 1 + \ln \sqrt{\det \gamma}.$$  

(2.52)

This slicing condition has become the standard for BBH simulations because, like maximal slicing [121, 160, 176], it has strong singularity avoidance properties. In other words, around the singularity, the lapse collapses to near zero, and proper time elapses more slowly, thus effectively avoiding any irregularity that the singularity could cause.

For the shift condition, we use a modified gamma-driver condition proposed by Alcubierre et al. [5],

$$\partial_0 \beta^i = \xi B^i,$$

$$\partial_0 B^i = \partial_0 \tilde{\Gamma}^i - \eta B^i,$$

(2.53)

where $\xi = 3/4$, and $\eta = 2/M$. Note that $\eta$ scales with the mass and therefore needs to be adjusted for unequal-mass systems. The term with $\eta$ is added to provide overall
stability and to remove high frequency coordinate noise.

The gauge can also be used to track the punctures throughout the computational domain by the shift:

$$\frac{dx^i}{dt} = -\beta^i.$$  \hspace{1cm} (2.54)

This simple ordinary differential equation is evolved along with the simulation in an implementation called \texttt{ShiftTracker} written by Andrew Knapp as a thorn for \texttt{MayaKranc}.

\section*{2.4 \texttt{MayaKranc}}

\texttt{MayaKranc} is the name of the PSU-GATech numerical relativity evolution code. Maya refers to the earlier code developed at Penn State in the early twenty-first century, and Kranc refers to the code generation package, \texttt{Kranc2BSSN}, (see Section 2.2) which generates Einstein’s Field Equations in 3+1 BSSN form in C. The code has been developed and improved over several years by Ian Hinder, Frank Herrmann, Tanja Bode, Eloise Bentivegna, Frank Knapp, and Roland Haas, and under the direction of Pablo Laguna and Deirdre Shoemaker. The code has several components that can be classified into a few categories: evolution equations, parallelization, mesh refinement, and calculations. The evolution equations were already discussed, and calculation thorns will be discussed in Chapter 3. Mesh refinement and parallelization are the last two topics for this chapter.

\textbf{Mesh Refinement and Carpet:} The computational domain of a BBH is very large with respect to the initial separation of the BHs for two reasons: to be able to extract waveforms far from the source and to avoid reflections from the boundary of the grid structure. Around a typical non-spinning BH with mass, $m = 0.5M$, grid spacings are on the order of $10^{-2}M$ or less. To have a full three-dimensional grid structure (with boundaries around $300M$) with this spacing is currently computationally unrealistic. The ideal grid structure would have an adaptive scheme, that is, when the BHs are far apart with little interaction between them, there is a lower resolution, and when they approach, the resolution increases. However, this technology also does not currently exist in a form usable for BBH simulations. Therefore, we must make a compromise and use an adaptive mesh refinement grid structure. This means that around each BH there are a series of different refinement levels, each with a different resolution and different size. There are two types of refinement levels: moving and fixed. Typical simulations have five or six moving refinement levels, with the highest resolution being centered around the BH and fully containing the BH horizon. These moving levels follow the BHs as they move (either by finding the minimum in $\chi$ or by Equation 2.54) and merge
Table 2.1. Grid structure for R1 test run, showing the grid spacing, resolution, number of points, and radius of each refinement level. Refinement level 0 has the highest resolution. Rows denoted with a * are moving grids and initially there are two such structures, each centered around one of the initial BHs.

<table>
<thead>
<tr>
<th>Grid</th>
<th>h</th>
<th>Resolution</th>
<th>Points/Radius</th>
<th>Radius</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.03875 M</td>
<td>M/25.8065</td>
<td>16</td>
<td>0.62 M</td>
</tr>
<tr>
<td>1</td>
<td>0.07750 M</td>
<td>M/12.9033</td>
<td>16</td>
<td>1.24 M</td>
</tr>
<tr>
<td>2</td>
<td>0.15500 M</td>
<td>M/ 6.4516</td>
<td>16</td>
<td>2.48 M</td>
</tr>
<tr>
<td>3</td>
<td>0.31000 M</td>
<td>M/ 3.2258</td>
<td>16</td>
<td>4.96 M</td>
</tr>
<tr>
<td>4</td>
<td>0.62000 M</td>
<td>M/ 1.6129</td>
<td>16</td>
<td>9.92 M</td>
</tr>
<tr>
<td>5</td>
<td>1.24000 M</td>
<td>M/ 0.8064</td>
<td>32</td>
<td>39.68 M</td>
</tr>
<tr>
<td>6</td>
<td>2.48000 M</td>
<td>M/ 0.4032</td>
<td>32</td>
<td>79.36 M</td>
</tr>
<tr>
<td>7</td>
<td>4.96000 M</td>
<td>M/ 0.2016</td>
<td>32</td>
<td>158.72 M</td>
</tr>
<tr>
<td>8</td>
<td>9.92000 M</td>
<td>M/ 0.1008</td>
<td>32</td>
<td>317.44 M</td>
</tr>
</tbody>
</table>

and separate with the binary’s separation. There are also three or four fixed refinement levels that are the largest in size, have lower resolutions, and are where wave extraction takes place. This refinement level infrastructure is provided by Carpet [60, 153] and has an implementation as a thorn for the Cactus infrastructure. The general structure of the grid uses a factor-of-2 resolution scheme, meaning each successive level has half the resolution of the one below it. Care must be taken when setting up the grids, since a certain resolution is needed to resolve the BHs on the finest refinement level as well as the gravitational radiation on the extraction level. Various symmetries can be invoked to reduce the computational cost. Several runs presented in this dissertation use $\pi$-symmetry and $\hat{z}$-reflection symmetry, reducing the number of points needed by four.

As an example to clearly illustrate a typical numerical grid setup, I present the grid structure of our R1 run. R1 is used to test the code when changes are made. R1 has nine levels of refinement, with the highest resolution $\sim M/26$, or in other words, there are 16 grid points over a ‘radius’ of 0.62M. The outer boundaries are at 317M and, thus, there is a total volume of $(634M)^3$ in the computational domain. Table 2.1 gives the details of each refinement level of the grid structure, the radius, total number of points in the radius, resolution, and grid spacing. Figure 2.1 is a two-dimensional representation of the grid structure for R1.

**Parallelization and Cactus:** Carpet is central to BBH simulations and despite some of its drawbacks the field of NR would not be as far advanced without it. Due to the size of the Carpet grid structures, most BBH simulations require several processors with many gigabytes of RAM available. Therefore, of equal importance to the field is parallelization software. This is provided for us by the Cactus infrastructure [48].
**Figure 2.1.** Moving grid structure for the R1 test run with no symmetries. As the simulation progresses, the grids move along with the BHs and subsequently merge as the BHs merge. Not shown in the figure are the fixed refinement levels.

*Cactus* has two parts, the flesh and the thorns. The flesh of *Cactus* binds all the thorns together and provides code for multi-process handling and scheduling. The thorns are the modules, which can contain code for calculations, storage, evolution, and so on. *Carpet* and *ShiftTracker* are both implemented as thorns. The *Kranc2BSSN* code generation package generates a thorn called *Kranc2BSSNChi*, which contains the BSSN evolution equations and gauge equations. Several calculation thorns are discussed in Chapter 3, including *Psi4Analysis*, *IHSpin*, *AHFinderDirect*, and *YlmDecomp*.

With the stable BSSN evolution equations, the ability to generate initial data that does not need excision, and gauge conditions that are both stable and avoid singularities, we are able to accurately evolve a BBH spacetime through inspiral, merger, ringdown, and indefinitely afterwards. In order to do this, we use the computational machinery provided by the mesh refinement of *Carpet* and the backbone of *Cactus*. However, this is all meaningless unless we are able to extract physically meaningfully data from the evolution. In the next chapter, I will detail how we calculate the final mass, spin, and kick velocity of the remnant BH. I will also discuss the waveform extraction techniques used and how this relates to the observable physical gravitational strain.
Chapter 3

Computing the Mass, Spin, and Kick of a Black Hole

There are two different approaches to calculating the mass, spin, and momenta of BHs. The first is a local approach, using horizon formulations of BHs to calculate the mass and spin from the local properties of the horizon. The second is a global approach, using concepts of conservation laws and the energy and momentum carried away by gravitational waves to make a deduction on the final mass and spin of the remnant BH. Both methods have their advantages and disadvantages. Local calculations tend to be more accurate, but are more computationally costly. Further, we do not have a local calculation of momentum currently implemented. With a global calculation, the final properties of the remaining BH can be calculated, including the kick velocity, but the properties of the original two BHs in the binary cannot. In this chapter, I will discuss both local and global calculations of mass, spin, and momentum, along with the drawbacks and error associated with each method.

3.1 Local Calculations

Knowing the location of the BH during the numerical simulation is important for two reasons. First, the region around the BH may need to be removed from the numerical grid for stability purposes. This is called excision. MayaKranc uses a Moving Puncture Recipe (see Section 2.3) where excision is not utilized. The second reason, and the reason why we locate the BH, is to measure the remnant BH’s physical quantities: the mass and spin.

The event horizon, the boundary between null rays that can escape to future infinity
and null rays that cannot, may seem like the obvious choice for finding the location of the BH. However, the event horizon is a global quantity, meaning a good part of the spacetime must be known before it can be found. For this reason, finding the event horizon can only be done after the simulation has ended. Therefore, an event horizon cannot be used to track the BHs in ‘real-time’ during the simulation. Other horizon concepts exist that, unlike the event horizon, are local and may be used to find the location on each spatial slice. These local horizons can be located at each time step of the simulation, have very useful properties for numerics, and have a notion of mass and spin. I will discuss two concepts of horizons in this section, *Apparent Horizons (AHs)* and *Isolated Horizons (IHs)*.

### 3.1.1 Local Calculation of Mass - Apparent Horizons

A marginally trapped surface (MTS) is defined as a spacelike two-dimensional surface embedded in the three-dimensional spatial slice, $\Sigma$, whose outgoing null geodesics have zero expansion, $\Theta$. This can be written as an elliptic equation in our $3 + 1$ variables [175],

$$\Theta := D_i s^i + K_{ij} s^i s^j - K = 0,$$

(3.1)

where $s^i$ is the unit normal to the MTS. An AH is then defined as the outermost MTS in $\Sigma$.

We use a direct elliptic solver, *ApparentHorizonFinderDirect (AHFDirect)*, which was developed simultaneously yet separately by Jonathon Thornburg [163] and Erik Schnetter [152]. Both were written as thorns for the Cactus infrastructure (see Section 2.4); however, Schnetter’s version was more easily integrable with *MayaKranc*, hence its inclusion in the current implementations. Given an initial guess, *AHFDirect* solves Equation 3.1 on our three-dimensional Cartesian grid. This method allows run speeds of up to 30 times faster than solvers that use other methods.

There are some very useful properties of AHs that we can make use of numerically. First, an AH is guaranteed (under the right conditions) to coincide or be contained within the event horizon. This assures that excision of coordinates within the AH will remove only parts of the spacetime that are causally disconnected from the region of interest. The AH coincides with the event horizon for stationary solutions. Therefore, early in the simulation when the BHs are far apart and after the BHs merge and the remnant settles down, we can use the area of the AH to calculate the irreducible mass of the BH,
Figure 3.1. Persistence of the two marginally trapped surfaces (red) after the common horizon (blue) forms. The black line indicates the trajectories of the marginally trapped surfaces. Horizons are from the R1 test run.

\[ M_{irr} = \sqrt{\frac{A}{16\pi}} \]  

(3.2)

At these phases of the evolution, the AH is an isolated horizon and therefore, the spin and horizon mass of the BHs can be calculated, as in the next section.

From Equation 3.1, it is clear that AH is gauge dependent. It is therefore possible to find a gauge where the AH does not exist. However, with the traditional numerical relativity gauge (see Section 2.3.3), this has yet to pose a problem in any of my simulations. Another possible problem is that AHDirect solves Equation 3.1, but this is the equation for a MTS and not an AH. It is possible that there are many nested MTSs for any given spacetime and therefore, choice of an initial guess for the AH finder is crucial. This only becomes an issue when trying to find the earliest common horizon that forms when the two BHs merge. Each individual BH has an AH that persists even after the formation of the common horizon (see Figure 3.1). In this case, we have nested MTSs and need to make sure our initial guess for the solver is appropriately chosen.
3.1.2 Local Calculation of Spin - Isolated Horizons

With apparent horizons, we can calculate the irreducible mass of the BHs in the system. However, this is only the final mass of the BH if the BH has zero spin. In general, the remnant BH will have some spin, even in the case of initially non-spinning BHs since not all of the initial angular momentum will be radiated. Therefore, it is absolutely essential to have a local calculation of the spin. Fortunately, there is a framework, the *isolated horizon formalism* recently developed by Ashtekar, Beetle, and Fairhurst [8], that can be implemented numerically to accomplish our goal. The isolated horizon formalism builds off of the concept of describing a BH by a “trapping horizon”, which was developed by Hayward [93]. The numerical implementation of isolated horizons was discussed by Dreyer, Krishnan, Shoemaker, and Schnetter [76].

Suppose we have a marginally trapped surface, $S$, on each spatial slice, $\Sigma$. A Non-expanding Horizon (NEH) is defined as a three-dimensional hypersurface, $\Delta$, foliated by these marginally trapped surfaces, that are topologically $S^2 \times \mathbb{R}$ and null. From the definition of MTS, the expansion of the NEH is $\theta(\ell) = q^{ab} \nabla_a \ell_b = 0$, where $q_{ab}$ is the induced 2-metric on $S$, and $\ell$ is any null normal to $\Delta$. An isolated horizon is then a NEH with added structure. Fortunately, the final mass and spin do not depend on the added structure, and therefore, we actually work with the concept of a NEH.

The angular momentum and mass of the BH is then derived via Hamiltonian methods. The marginally trapped surface, $S$, is axisymmetric, that is, it has a rotational Killing vector field $\vec{\varphi}$ that satisfies

$$\mathcal{L}_{\vec{\varphi}} q_{ab} = 0. \quad (3.3)$$

The magnitude of the angular momentum of the BH is then

$$J_\Delta = \frac{1}{8\pi} \oint_S \varphi^a s^b K_{ab} dA, \quad (3.4)$$

where $s^a$ is the outward pointing normal to $S$, and $K_{ab}$ is the extrinsic curvature of our spatial slice, $\Sigma$. This equation is very similar to the equation for $J_{adm}$, with the main difference being that this integral is taken over the surface, $S$, whereas the $J_{adm}$ calculation is taken at infinity.

With the spin of the BH and the irreducible mass calculated from the apparent horizon area via Equation 3.2, we can now calculate the mass of the BH:
This equation is known as Christodoulou’s equation, as it was derived earlier via a different method [63].

The isolated horizon formalism is relevant to our simulations for very early and late times when our BHs are approximately stationary. For stationary BHs, it is easy to see that the world tube of AHs will necessarily be a NEH. Therefore, Equations 3.4 and 3.5 can be used to find the spin and mass. In the final stages of inspiral, merger, and ringdown, there are large amounts of radiation being emitted and entering our MTSs. Therefore, we no longer can use the IH formalism in this regime, since the world tubes will be spacelike rather than null. Fortunately, for this situation, another “horizon” formalism has been developed by Ashtekar and Krishnan [9], the dynamical horizon formalism. This formalism is very similar to the isolated horizon formalism, but allows for non-stationary BHs.

Even though the isolated horizon formalism is powerful, we do not implement it fully since it is computationally expensive to find the NEH and its associated Killing field \( \vec{\varphi} \). However, we do calculate the AH with an approximate Killing vector at each spatial slice by using Campanelli et al.’s coordinate angular momenta [57]

\[
\begin{align*}
\varphi_x &= (0, -\hat{z}, \hat{y}), \\
\varphi_y &= (\hat{z}, 0, -\hat{x}), \\
\varphi_z &= (-\hat{y}, \hat{x}, 0),
\end{align*}
\]

and Equations 3.4 and 3.5 on the AH surface to calculate the mass and spin. Campanelli’s \( \varphi \) allows us to give the horizon an orientation, with \( x, y, \) and \( z \) components. This method shows good agreement in the spin when compared to actually calculating the Killing field associated with the horizon [57]. Further, Herrmann et al. [99] calculates the spin on a spherical surface situated where the AH is expected, without finding the AH, and finds approximately the same spin until merger. In all spins quoted hereafter, we find the AH and use Campanelli’s \( \varphi \) to calculate the isolated horizon spin on the AH surface.
3.2 Global Calculations

If we were able to calculate the amount of energy, momentum, and angular momentum that is leaving the system through gravitational waves, we would be able to use conservation laws to calculate the final parameters of our BH. Therefore, it is crucial to have an accurate and coordinate-independent notion of the gravitational wave content of our system. From the initial data, the initial ADM energy, $M_{\text{adm}}$, and initial angular momentum $\vec{J}_{\text{init}} = \vec{L}_{\text{init}} + \vec{S}_{\text{init}}$ are known, where $\vec{L}_{\text{init}}$ and $\vec{S}_{\text{init}}$ are the initial orbital angular momentum and spin, respectively. The initial linear momentum, $\vec{P}_{\text{init}} = \vec{P}_+ + \vec{P}_-$ is always configured to be zero. With this, we can write our conservation of energy and momenta as

\begin{align}
M_f &= M_{\text{adm}} - E_{\text{rad}}, \\
\vec{P}_{\text{kick}} &= -\vec{P}_{\text{rad}}, \\
\vec{J}_f &= \vec{J}_{\text{init}} - \vec{J}_{\text{rad}},
\end{align}

where $M_f$, $\vec{P}_{\text{kick}}$, and $\vec{J}_f$ are the final energy, momentum, and angular momentum of the remnant BH, and $E_{\text{rad}}$, $\vec{P}_{\text{rad}}$, and $\vec{J}_{\text{rad}}$ are the energy, momentum, and angular momentum carried away by gravitational radiation, respectively.

In this section, I will discuss how we characterize the gravitational wave content of our system through the Newman-Penrose formalism and the fourth Weyl Scalar, how this scalar relates to the gravitational strain, and how we calculate the radiated quantities.

3.2.1 Waveform Extraction and Decomposition

The Newman-Penrose formalism [61, 133] uses a null tetrad to calculate various scalars, one of which is related to the gravitational wave content of asymptotic spacetimes. The tetrad consists of four basis vectors, \{\(l^\mu, n^\mu, m^\mu, \bar{m}^\mu\}\}, where \(l^\mu\) and \(n^\mu\) are real, \(m^\mu\) and \(\bar{m}^\mu\) are imaginary, and \(\bar{m}^\mu\) is the complex conjugate of \(m^\mu\). The vectors must satisfy orthogonality relations,

\begin{align}
l^\mu l_\mu &= n^\mu n_\mu = m^\mu m_\mu = \bar{m}_\mu \bar{m}^\mu = 0, \\
m^\mu l_\mu &= \bar{m}^\mu l_\mu = m^\mu n_\mu = \bar{m}^\mu n_\mu = 0,
\end{align}

where $l_\mu$, $n_\mu$, $m_\mu$, and $\bar{m}_\mu$ are the contravariant vectors corresponding to the covariant basis vectors $l^\mu$, $n^\mu$, $m^\mu$, and $\bar{m}^\mu$, respectively.
in addition to a normalization requirement,

$$n^\mu n_\mu = -\bar{m}^\mu m_\mu = 1. \quad (3.14)$$

We choose a “quasi-Kinnersley” [50] null tetrad:

$$l^\mu = \frac{1}{\sqrt{2}}(n^\mu + r^\mu), \quad (3.15)$$

$$n^\mu = \frac{1}{\sqrt{2}}(n^\mu - r^\mu), \quad (3.16)$$

$$m^\mu = \frac{1}{\sqrt{2}}(\theta^\mu + i\phi^\mu), \quad (3.17)$$

where $n^\mu$ is the unit normal to the hypersurface and $\{r^\mu, \theta^\mu, \phi^\mu\}$ are the unit vectors of spherical coordinates.

Once the tetrad is chosen, we project the completely anti-symmetric Riemann curvature tensor, or the Weyl tensor [170], $C_{\alpha\beta\gamma\delta}$, using the tetrad basis vectors to construct scalars. These scalars are not true scalars because they vary under a rotation of the tetrad. The scalar used to encapsulate the wave content is denoted by $\Psi_4$ and is

$$\Psi_4 = C_{\alpha\beta\gamma\delta} n^\alpha m^\beta n^\gamma \bar{m}^\delta. \quad (3.18)$$

The scalar, $\Psi_4$, is a spin-weight $-2$ pseudoscalar and can be decomposed into spin-weight $-2$ spherical harmonics (see [149] Appendix A for a thorough discussion of spin-weighted spherical harmonics). Physically this is useful because it has been shown that the final kick of a black hole due to asymmetries in either mass or spin is due to specific mode contributions [98]. Quasi-normal mode analysis also uses the modal decomposition of $\Psi_4$ to calculate the final mass and spin from the ringdown waveform [27]. $\Psi_4$ can be decomposed as a sum of a coefficient times the spherical harmonics, $Y_{\ell m}(\theta, \phi)$:

$$\Psi_4 = \sum_{\ell=2}^{\infty} \sum_{m=-\ell}^{\ell} C_{\ell m}(t, r) Y_{\ell m}(\theta, \phi). \quad (3.19)$$

The coefficients, $C_{\ell m}(t, r)$, contain all of the time dependence of the gravitational waveform and, by the peeling theorem, should have $1/r$ dependence. We can calculate the coefficients, $C_{\ell m}$, using orthogonality of the spin-weighted spherical harmonics:

$$C_{\ell m}(t, r) = \int \Psi_4 Y_{\ell m}(\theta, \phi) d\Omega, \quad (3.20)$$
where the integral is taken over a 2-sphere with solid angle \( d\Omega \).

We are interested in the gravitational waveform at infinity but we are limited by the finite size of our numerical grid. Therefore, we calculate \( C_{lm} \) at finite extraction radii and extrapolate to infinity. Two thorns called \texttt{WeylScalar4} and \texttt{YlmDecomp} for \texttt{MayaKranc} are used. \texttt{WeylScalar4} calculates \( \Psi_4 \) at each grid point in our computational domain. \texttt{YlmDecomp} was written by Tanja Bode and interpolates \( \Psi_4 \) onto a sphere of finite extraction radii, and calculates \( C_{lm} \) as in Equation 3.20 at each time step (or every \( N \) time steps).

The extrapolation to infinity introduces error and is one the drawbacks of using \( \Psi_4 \) to calculate the final mass and spin of the system. In addition, when choosing extraction radii, one must be very careful not to be ‘too close’ to the binary system or have detectors that span different refinement levels. Since subsequent levels of the grid structure have a staggered resolution scheme, the error in the coarser resolution grid will be larger than the finer grid, and thus the extrapolation will be difficult since the waveforms are not consistent. We have to fine tune the grid so that the extraction radii are all on the same refinement level, have sufficient resolution for accuracy, and are far enough away that the peeling theorem is applicable. This typically leads to a range of 50M - 100M for the extraction level.

### 3.2.2 Radiated Energy, Momentum, and Angular Momentum

The Weyl Scalar, \( \Psi_4 \), describes the outgoing gravitational radiation in an asymptotically flat spacetime but is not physically useful. However, it is related to the gravitational strain,

\[
\Psi_4 = \ddot{h}_+ - i\dot{h}_x, \tag{3.21}
\]

where \( h_+ \) and \( h_x \) are the two polarizations of gravitational radiation and a dot represents a time derivative. The strain is very important physically because this is the quantity that will be directly observed at gravitational wave detectors such as LIGO and LISA. The strain and its first derivative will also be vital to the calculation of the radiated energy, momentum, and angular momentum of the BBH system.

To find the expressions for the radiated quantities, the full spacetime metric is taken to be flat plus a small perturbation, \( g_{\mu\nu} = \delta_{\mu\nu} + h_{\mu\nu} \). The gauge is chosen so that the small perturbation, \( h_{\mu\nu} \), is transverse and traceless (TT). The Isaacson Stress-Energy tensor is constructed [130] and from it the energy flux, momentum flux, and angular momentum flux can be found. The equation for the time derivative of the radiated
Figure 3.2. \(\Psi_4\) (top panel) and \(h\) with integration constants removed (bottom panel). In each panel, the real (red), imaginary (blue) and magnitudes (black) are plotted. Note the unphysical spurious radiation at the beginning of the waveform. Waveforms are from the R1 test run.

quantities in terms of \(\Psi_4\) are:

\[
\frac{dE}{dt} = \lim_{r\to\infty} \frac{r^2}{16\pi} \int \int_{-\infty}^{t'} \int_{-\infty}^{t'} dt'' \Psi_4^2 d\Omega, \tag{3.22}
\]

\[
\frac{dP^i}{dt} = \lim_{r\to\infty} \frac{r^2}{16\pi} \int \left[ \left( \int_{-\infty}^{t'} dt' \Psi_4 \right) \times \hat{j}_i \left( \int_{-\infty}^{t'} dt' \int_{-\infty}^{t''} \Psi_4 d\Omega \right) \right] d\Omega, \tag{3.23}
\]

\[
\frac{dJ^i}{dt} = \lim_{r\to\infty} \frac{r^2}{16\pi} \Re \left[ \Phi \left( \int_{-\infty}^{t'} dt' \Psi_4 \right) \times \hat{j}_i \left( \int_{-\infty}^{t'} dt' \int_{-\infty}^{t''} \Psi_4 d\Omega \right) \right] \tag{3.24}
\]

The equations for \(dE/dt\) and \(dP^i/dt\) differ by the directional operator, \(n^i = (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta)\) and the angular momentum operators in Equation 3.24 are

\[
\hat{\mathbf{j}}_x = -\sin \varphi \partial_{\theta} - \cos \varphi \left( \cot \theta \partial_{\varphi} + 2i \csc \theta \right), \tag{3.25}
\]

\[
\hat{\mathbf{j}}_y = \cos \varphi \partial_{\theta} - \sin \varphi \left( \cot \theta \partial_{\varphi} + 2i \csc \theta \right), \tag{3.26}
\]

\[
\hat{\mathbf{j}}_z = \partial_{\varphi}. \tag{3.27}
\]

A thorn called \texttt{Psi4Analysis} written by Frank Herrmann calculates the three equations
above on an extraction sphere at finite radii. Simpson’s method is used to integrate the equations to obtain $E_{rad}$, $P_{rad}$, and $J_{rad}$.

The main drawback to calculating $E_{rad}$, $P_{rad}$, and $J_{rad}$ during the evolution is the integration constant (discussed below). Therefore, we need a method to calculate the radiated quantities in post-processing where the integration constant can be removed. We can use the properties of spherical harmonics and the modal decomposition (Equation 3.19) in summation form to rewrite Equations 3.22 and 3.23 in terms of the mode overlaps. Defining the mode overlap, $\langle \ell, m | \ell', m' \rangle$, as

$$\langle \ell, m | \ell', m' \rangle = \frac{1}{16\pi} \text{Re} \left\{ \overline{B}_{\ell m'} B_{\ell m} \int Y_{\ell' m'} Y_{\ell m} n^\mu d\Omega \right\}, \quad (3.28)$$

with $n^\mu = (1, n^i)$ and $\mathcal{B}_{\ell m} = \int_{-\infty}^{t} dt' C_{\ell m}$, the time derivative of the four-momentum is

$$\frac{dP^\mu}{dt} = \sum_{\ell m \ell' m'} \langle \ell, m | \ell', m' \rangle . \quad (3.29)$$

The 0 component of Equation 3.29 is $dE/dt$ while the 1, 2, and 3 components are the three components of $dP^i/dt$. From this equation and the properties of spin-weight spherical harmonics, it is clear that only certain mode overlaps can contribute to the radiated energy and momentum. For example, in $dE/dt$ the integral $\int -2 \tilde{Y}_{\ell' m'} -2 Y_{\ell m} n^\mu d\Omega = 0$ unless $\ell = \ell'$ and $m = m'$ by orthogonality. Therefore, the only contributions to the radiated energy come from the overlap of the mode with itself. This is not true for all components of the radiated momentum however. The $\varphi$ dependence of the spherical harmonics is $e^{im\varphi}$ and therefore, in the $x$ and $y$ component of $dP^i/dt$ there is an extra factor of $\cos \varphi$ or $\sin \varphi$. This leads to the only contributing factors to $dP^x/dt$ and $dP^y/dt$ coming from mode overlaps where $m' = m \pm 1$. For $dP^z/dt$, there is no extra factor of $\varphi$ in the angular integral, so $m' = m$. The normal, $n^i$, also adds $\theta$ dependence to the angular integral, complicating the conditions on $\ell$. This method to calculate the radiated quantities from $\Psi_4$ from the specific mode contributions in post-processing is summarized by Ruiz et al. [149].

Within Equations 3.22 – 3.24, there is an integral $\int_{-\infty}^{t} \Psi_4 dt'$. We do not have $\Psi_4$ over these integration limits, but only have $\Psi_4$ from $t_{min} = 0$. In other words, the gravitational wave content of the system is not known prior to the start of the simulation but is needed in the calculation of radiated quantities. This leads to the introduction of an integration constant:

$$\int_{-\infty}^{t} \Psi_4 dt' = \int_{0}^{t} \Psi_4 dt' + C . \quad (3.30)$$
This integration constant, $C$, can not be determined during the evolution of the system and must be determined after the fact. If it is not removed, the strain will drift off linearly since calculating $h$ from $\Psi_4$ includes two integrals and thus two integration constants. To remove the integration constant, we calculate the two integrals of $\Psi_4$ to find

$$h = \int_{-\infty}^{t} \int_{-\infty}^{t'} \Psi_4 dt' = \int_{0}^{t} \int_{0}^{t'} \Psi_4 dt' + C_1 t + C_2,$$

(3.31)

and fit a line to the strain. The linear dependence is then removed by subtraction. Calculations of the radiated quantities via post-processing can now occur, effectively removing the error introduced from the integration constants.

As mentioned in Section 2.3.1, the initial data contains spurious unphysical radiation that is not generated by the BBH system and is an artifact of the generation of the initial data. This spurious radiation must be removed in post-processing before calculating the radiated quantities. However, in some cases, merger occurs quickly, and the physical radiation and spurious radiation are superimposed. In this case, a local calculation is essential to getting accurate values for mass and spin.

From the gravitational radiation, the ability to calculate the radiated quantities allows a global calculation of the final mass, spin, and kick of the remnant black hole. A method to calculate these radiated quantities via $\Psi_4$ is available during the evolution of the spacetime and after the fact in post-processing, and there are methods to remove errors introduced by integration constants and spurious radiation. However, due to the fact that the radiation has to be extracted at distances far away from the BH and the refinement mesh uses a staggered resolution scheme, the mass and spin calculated via this global calculation is generally less accurate than those calculated via horizon methods. There is a quasi-local formulation for the linear momentum [116] but it is not currently implemented in MayaKranc and therefore, we resort to measuring the kick via $\Psi_4$. 
Chapter 4

Superkicks in Hyperbolic Encounters of Binary Black Holes

Numerical relativity estimates of the gravitational recoil or kick inflicted on the final BH from generic inspirals and mergers of BBH have triggered tremendous excitement in astrophysics. This is mainly due to the fact that most galaxies host a supermassive black hole (SMBH) at their centers [73, 148]. As galaxies merge, a kick to the final BH from the coalescence of the BHs at the galactic cores could have profound implications in subsequent mergers, affecting the growth of SMBHs via mergers as well as the population of galaxies containing SMBHs. In addition, there have been several suggestions of direct observational signatures of putative BH recoils [33, 74, 112, 123, 125, 157]. One study [113] presents evidence for the first candidate of a recoiling SMBH, however, there may be other explanations for the evidence [35, 75].

BH kick velocities depend on the mass ratio and spins of the merging BHs as well as on the initial configuration and subsequent dynamics of the binary. Studies published to date have been concerned with the most astrophysically relevant configuration, that of quasi-circular inspirals [85, 97, 98, 115]. Any asymmetry in the initial configuration of the BBH system, whether originating from different mass BHs or different spin configurations, will lead to asymmetric gravitational radiation resulting in a kick to the remnant BH. Analytic equations for kick velocities from quasi-circular systems were found by extrapolating the NR results [58], allowing us to examine each asymmetry contribution separately. The three contributions are (1) the kick from an asymmetry in the masses, $v_m$, (2) the kick parallel to the orbital angular momentum from the in-plane spin discrepancy, $v_s^\parallel$, and (3) the in-plane kick from the spins parallel to the orbital angular
momentum, \( v_s^\perp \). The total recoil velocity and the three contributions are [58, 144]

\[
\vec{V}_{\text{recoil}}(q, \vec{a}) = v_m \hat{e}_1 + v_s^\perp (\cos(\xi) \hat{e}_1 + \sin(\xi) \hat{e}_2) + v_s^\parallel \hat{e}_z,
\]

(4.1)

\[
v_m = A q^2 (1 - q) \left( 1 + B \frac{q}{(1 + q)^2} \right),
\]

(4.2)

\[
v_s^\perp = \frac{q^2}{(1 + q)^5} \left[ C \left( a_2^\parallel - qa_1^\parallel \right) + D \left( a_1^\parallel \right)^2 - q^2 \left( a_2^\parallel \right)^2 \right],
\]

(4.3)

\[
v_s^\parallel = K \cos(\Phi - \Phi_0) \frac{q^2}{(1 + q)^5} (a_2^\perp - qa_1^\perp),
\]

(4.4)

where \( A = 12,000 \text{ km s}^{-1} \), \( B = -0.93 \), \( C = 7,040 \text{ km s}^{-1} \), \( D = 1,460 \text{ km s}^{-1} \), \( K = 60,000 \text{ km s}^{-1} \), \( q \) is the mass ratio, \( q = m_1/m_2 < 1 \), \( a_i = \vec{S}_i/m_i^2 \) and ranges from 0 to 1. The quantities, \( a_i^\perp \) and \( a_i^\parallel \), are the components of the spin perpendicular and parallel to the initial orbital angular momentum, respectively. The angle \( \xi \) is the angle between the mass and spin contributions within the orbital plane, and the angle \( \Phi \) is related to the spin orientations when the black holes merge. First, note that any mass ratio other than 1 or 0 leads to a kick in the orbital plane, with a maximum \( v_m \sim 175 \text{ km s}^{-1} \) for \( q \approx 0.362 \). Secondly, to obtain a kick in the orbital plane from the spin, there must be a component of the spin parallel to the orbital angular momentum. The maximum contribution from this term is \( v_s^\perp \sim 450 \text{ km s}^{-1} \) for \( a_1^\parallel = a_2^\parallel = 1 \) for equal-mass BHs.

The kick in both these cases is generated within the orbital plane due to the symmetry of the system.

One remarkable discovery has been kicks of a few thousand km s\(^{-1}\) found in configurations of equal-mass binaries with initially anti-aligned spins in the orbital plane [51, 59, 83]. For near Bowen-York extremal spins \((a/m = 0.925)\), recoils as large as 3,300 km s\(^{-1}\) have been computed [65]. These “superkick” values can be understood by looking at the last equation above. The kick parallel to the orbital angular momentum is fully determined by the in-plane spin and has a maximum for \( \vec{a}_1^\perp = -\vec{a}_2^\perp = \hat{e}_x \), where \( \hat{e}_x \) is the component perpendicular to the initial momentum, \( \hat{e}_y \). When \( \cos(\Phi - \Phi_0) = 1 \) there is a maximum in the kick, \( v_s^\parallel \sim 3750 \text{ km s}^{-1} \). For spins within the orbital plane and no other asymmetries present, as long as the spins are anti-aligned with each other, the system exhibits \( \pi \)-symmetry, that is, \( \phi = \phi + \pi \). Therefore, a kick within the orbital plane is prohibited, resulting in all the kick in the \( \hat{z} \)-direction. However, if the spins are not anti-aligned in the orbital plane, there will be no symmetry in the system, and we expect to find both kicks within the orbital plane and parallel to the orbital angular momentum. This is a situation not taken into account by the analytic formula for the
kicks above.

In this chapter, we present the first extension of gravitational recoil to hyperbolic encounters. There are crucial differences between hyperbolic and quasi-circular configurations that affect the kick to the final BH. For quasi-circular orbits, the emitted radiation is asymmetrically beamed, and carries linear momentum with it. It tends to average out during the inspiral [32], producing a modest wobbling and drift of the center of mass of the binary. The final kick arises because as the binary approaches the plunge, the averaging loses its effectiveness, leading to a gradual recoil build-up. Both numerical simulations and post-Newtonian studies [32, 67] have confirmed the gradual kick accumulation during the inspiral, and, in addition, the studies have shown that most of the recoil is generated during the plunge. In some instances, during the plunge and ring-down there is also a period of anti-kick before reaching the final kick value [12, 155, 167].

The main motivation for this study was to consider plunge-dominated configurations to investigate whether kicks comparable to those for quasi-circular inspirals can be found. Surprisingly, we find that kicks larger than 4000 km s$^{-1}$ are in general produced for spin configurations equivalent to those studied in quasi-circular inspirals. We show below a configuration giving kick velocities as large as 10,000 km s$^{-1}$. Two qualitative features of hyperbolic encounters contribute to these larger kicks. Not only are hyperbolic encounters plunge-dominated, but the nature of the plunge is such that it enhances the beaming of radiated linear momentum [129].

The work presented in this chapter has been published in Physical Review Letters, 102:041101 [94].

4.1 Computational Infrastructure and Setup

We use a BSSN code, MayaKranc, with moving puncture gauge conditions and initiated with Bowen-York initial data as discussed in Chapter 2. The initial data consist of two equal-mass BHs with masses $m = M/2$ located along the $x$-axis: BH$_{\pm}$ is located at $x = \pm 5M$ and has linear momentum $\vec{P}_\pm = (\mp P \cos \theta, \pm P \sin \theta, 0)$ with $\theta$ the angle in the orbital plane between the momentum vector and the vector that connects the two BHs. The total initial orbital angular momentum is then $\vec{L}/M^2 = 10 (P/M) \sin \theta \hat{z}$. The spins of each BH are in the orbital plane: BH$_{\pm}$ has spin $\vec{S}_\pm = \pm (S \cos \phi_\pm, S \sin \phi_\pm, 0)$, with $\phi_\pm$ the angle in the orbital plane with respect to the $\pm x$-axis. The parameter space of our encounters is quite large: $\{P, \theta, S, \phi_\pm\}$. However, from exploratory runs we have gained a good understanding of the parameter space and isolated those parameters that
can be kept fixed without seriously compromising the goals of the study.

Kicks are computed from a surface integral [52, 134] involving the Weyl curvature
tensor $\Psi_4$ as in Section 3.2.2. Unless explicitly noted, all the reported kick velocities and
energy radiated were obtained from simulations with resolution $h = M/0.8$ on the mesh
used for the kick computation. Every run had 10 levels of factor-of-2 refinement, with
outer boundaries at $\sim 320M$. We discuss below the convergence of kick estimates as
the grid spacing is decreased and the extraction radius is increased as well as the error
associated with extrapolating the kick values to infinity. The estimated errors in all the
kick results presented here due to the finite differencing grid spacing $h = M/0.8$ and
extrapolation $r \to \infty$ are of the order of a few hundred km s$^{-1}$.

For most of the runs, we have kept the spin magnitudes at $S_\pm/M^2 = 0.2$ ($a/m = 0.8$),
with the exception of those runs used to investigate the dependence of the kick on $S$. We
kept fixed also the impact angle at $\theta = 26.565^\circ$. Finally, for most cases we kept the spin
direction of BH$-$ located at $x = -5M$ fixed at $\phi_- = 0^\circ$ or $45^\circ$. Once other parameters
were fixed from among a small set of values, the parameter we varied in general was
the linear momentum magnitude $P$. To investigate the $\phi$ dependence of the kick, we set
$\phi_- = \phi_+ = \phi$ and varied $\phi$ for constant $P$.

### 4.2 Results

We begin by keeping $\phi_-\,$ fixed and vary the initial orbital angular momentum for three
different values of $\phi_+$. Table 4.1 gives the components of the recoil along the initial
orbital angular momentum, $V_\parallel$, and in the initial orbital plane, $V_\perp$, in km s$^{-1}$ (and the
total recoil $V$). Notice that the largest recoil in this case happens when $\phi_+ = 45^\circ$.

Another important observation is that, although the dominant component of the kick is
$V_\parallel$, as we increase $\phi_+$ a substantial component of the kick is also generated in the orbital
plane (see $V_\perp$). An in-plane kick is expected since spins in the orbital plane that are
not anti-aligned with each other break the rotational symmetry of the system. However,
this configuration does not seem to be accounted for in the quasi-circular equation for
the in-plane kick, Equation 4.3. The rightmost column in Table 4.1 gives the $r \to \infty$
extrapolated radiated energy as a percentage of the total initial energy of the binary.

We see that increasing the angular momentum increases the energy radiated, up to very
substantial values, as large as 13%.

**Spin Dependence:** For the case $P/M = 0.2665, \phi_+ = 45^\circ$ in Table 4.1, we have carried
out simulations to investigate the dependence of the kick with the initial BH spins ($a/m$).
Table 4.1. Configuration parameters $P/M$, $\phi_+$ and initial orbital angular momentum $L/M^2$ for the cases with $\phi_- = 0^\circ$ and $S_+/M^2 = 0.2$. The last four columns show the corresponding kick velocities of the final BH in km s$^{-1}$ as well as the % of energy radiated.

| $P/M$ | $\phi_+$ | $L/M^2$ | $V_\parallel$ | $V_\perp$ | $V$ | $E_{\text{rad}}$ |%
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Figure 4.1. Magnitude of the kick velocity as a function of the magnitude of the initial BH spin ($a/m$) for the case ($P/M = 0.2665, \phi_+ = 45^\circ$)
Figure 4.2. Kick velocity $V_\parallel$ as a function of $\alpha = 180^\circ - \theta - \phi$ for the cases with spin orientation $\phi_+ = \phi_- = \phi$ and initial linear momentum $P/M = 0.3075$, corresponding to initial angular momentum $L/M^2 = 1.275$. The solid line represents the fit $V_\parallel = -10,256 \cos(\alpha + 86^\circ)$ km s$^{-1}$.

We increase the initial spin from $a/m = 0.2$ to $a/m = 0.8$. Simulations of spins greater than $a/m = 0.8$ require very fine resolutions around the BHs or they artificially radiate angular momentum and are therefore very costly computationally [128]. The results are displayed in Figure 4.1. We find that, to first order, the kick is proportional to $a/m$, as found in quasi-circular orbits [98]. However, as the initial spin of the BHs grows, we found hints of the quadratic spin dependence also obtained in quasi-circular orbits [139].

$\alpha$ Dependence:

The configuration we have found to yield the largest kick has the spins anti-aligned $\phi_+ = \phi_- = \phi$, as in the case of quasi-circular orbits [51, 59, 83], and initial linear momentum $P/M = 0.3075$, corresponding to initial angular momentum $L/M^2 = 1.275$. The kicks are essentially along the direction of the initial orbital angular momentum, the $\hat{z}$ direction. We set $\phi_+ = \phi_- = \phi$ and vary $\phi$ from $0^\circ$ to $360^\circ$. Figure 4.2 shows the kick velocity $V_\parallel$ as a function of $\alpha = \theta - \phi$, where $\alpha$ measures the angle between the initial spin and linear momentum vectors. The solid line represents the fit $V_\parallel = -10,256 \cos(\alpha + 86^\circ)$ km s$^{-1}$ obtained via a least squares fitting algorithm. This is the same angular dependence found in quasi-circular orbits [59] and Equation 4.4. Furthermore, as with
circular inspirals, the maximum kick is obtained for $\alpha \approx 90^\circ$ although in these hyperbolic encounters the kick is significantly larger, close to 10,000 km s$^{-1}$.

**Angular Momentum Dependence:**

To investigate the dependence on the initial orbital angular momentum, we selected the case $\phi_+ = \phi_- = \phi = 45^\circ$ or $\alpha = 108^\circ$ in Figure 4.2, which yields a kick magnitude of 9,589 km s$^{-1}$ and 15% energy radiated, and carried out simulations varying the initial momentum of the BHs. Figure 4.3 shows the magnitude of the kick velocity $V$ (top panel) and the energy radiated $E_{\text{rad}}$ in % of the initial energy (bottom panel) as a function of $L/M^2$. Note that the maximum of $V$ does not occur for maximum $E_{\text{rad}}$. This is the same behavior seen in Table 4.1 for the three different values of $\phi_+$.

The case with the largest initial angular momentum, $L/M^2 = 1.375$, has an interesting feature as displayed in the top panel of Figure 4.4. There is a pronounced *anti-kick* before the recoil reaches its final value. In other words, there is a period of beamed linear momentum radiated in one direction followed by another period of beamed radiation in the opposite direction. The reason for this anti-kick could be due to the fact that the plunge is not as pronounced, appearing more *circular-like*. That is, there is a decrease in the rate at which the binary comes together, as one can see in the bottom panel of
Figure 4.4. Accumulation of the kick velocity extracted at $r = 75 \, M$ (top panel) and binary separation (bottom panel) as a function of time for the case $L/M^2 = 1.375, \phi_+ = \phi_- = 45^\circ$ (red) in Figure 4.3 compared to $L/M^2 = 1.225, \phi_+ = \phi_- = 45^\circ$ (blue) which exhibits no anti-kick.

Figure 4.4 during the time interval $20 - 40 \, M$. Thus, the flux vectors responsible for the kick have more time to undergo the phase shift needed for the appearance of an anti-kick [155].

Since a kick is caused by asymmetrical gravitational wave emission, we can investigate the anti-kick in another way, by looking at mode contributions of $\Psi_4$. The dominant contributions to the kick in the $\hat{z}$-direction are from the overlap of $l = 2, m = 2$ and $l = 2, m = -2$ modes of $\Psi_4$ with themselves [43]. From Equation 3.28, we see that the contribution to the kick depends on the first integral of $C_{\ell m}$ and the angular contribution from the spherical harmonics. The angular part of the equation is equal and opposite for $\langle 2, 2 | 2, 2 \rangle$ and $\langle 2, -2 | 2, -2 \rangle$ and therefore if $C_{\ell m}$ are the same for both of those modes, there is no contribution to the kick since they exactly cancel. For cases with no anti-kick, in general, one of $C_{22}$ or $C_{2,-2}$ dominates the other, leading to asymmetrically beamed gravitational radiation. For the anti-kick illustrated in Figure 4.4, $C_{2,-2}$ dominates during the more circular like part of the orbit, and then $C_{22}$ begins to dominate during the plunge and ringdown. Therefore, there are two distinct periods of radiation in opposite directions leading to the anti-kick. This is depicted in the top panel of Figure 4.5.
Convergence and Error Analysis: Although strictly speaking the kick formula (Equation 3.23) must be evaluated in the limit $r \to \infty$, we applied it at extraction radii $r/M = \{40, 50, 75, 85, 100\}$. To get an estimate of the error due to the extrapolation to infinity, we take the kick to be

$$V(r) = V_\infty + K_0/r + O(r^{-2}) .$$

The resultant kicks were fitted to both $V(r) = V_\infty^{(1)} + K_0/r$ and $V(r) = V_\infty^{(2)} + K_1/r + K_2/r^2$. The extrapolated $r \to \infty$ kicks and their errors were estimated from

$$V_\infty = \frac{(V_\infty^{(1)} + V_\infty^{(2)})}{2},$$

$$\delta V_\infty = |V_\infty^{(1)} - V_\infty^{(2)}|,$$

respectively.

In addition to the errors from extracting the gravitational recoil at a finite radius, the values of the kicks are affected by numerical finite differencing resolution. To investigate
Figure 4.6. Magnitude of the kick velocity as a function of the extraction radius for different resolutions in the case \( P/M = 0.2665, \phi_+ = 45^\circ \). From bottom to top are respectively resolutions of \( h = \{ M/0.4, M/0.5, M/0.63, M/0.8 \} \) at the extraction level. Dots are the data and lines correspond to the fit \( V(r) = V^{(2)}_\infty + (K_1/r + K_2/r^2) \).

To estimate these errors, we selected the case \( P/M = 0.2665, \phi_+ = 45^\circ \) from Table 4.1 and carried out simulations with a series of resolutions \( h = \{ M/0.4, M/0.5, M/0.63, M/0.8 \} \) on the extraction level. Figure 4.6 shows the data (points) and the corresponding fitting (lines) to \( V(r) = V^{(2)}_\infty + K_1/r + K_2/r^2 \). We estimate the error in the kicks due to finite differencing resolution to be of the form

\[
V_h = V + Ch^d
\]  

(4.8)

where \( V \) is the actual value of the final kick, \( d \) is the order of convergence, and \( Ch^d \) is the estimated error. We would expect to find \( d \) to be around 4, since our code is fourth order accurate. However, due to lower order accurate parts of the code (for example, second order interpolation of functions at refinement boundaries), we expect to obtain an order of convergence less than fourth. We then use Richardson Extrapolation with the three highest values of grid spacing, \( h \), to find \( V, C \), and \( d \). We find that at a given extraction radius, the error in the kick scales as \( h^3 \), and the kick itself grows with resolution. Based on this \( h^3 \) behavior, we estimate the error in the kick extrapolated as \( r \to \infty \) computed
using $h = M/0.8$ to be of the order of a few hundred km s$^{-1}$, and we expect all the kicks presented to be of a similar accuracy.

**Conclusions:** We have carried out a study of the gravitational recoil of the final BH in the merger of hyperbolic BBH encounters. We have found that in general the kick velocities for in-plane initial BH spins are significantly larger than those from the corresponding quasi-circular mergers. Our results suggest that kicks as large as 10,000 km s$^{-1}$ are possible. We have also found that the dependence of the kick on the initial magnitude of the BH’s spins is similar to the quasi-circular case. We have found cases which exhibit a strong anti-kick for large initial angular momentum. As we increase the initial angular momentum for a given fixed $\phi$, $\theta$, and spin configuration, the final kick increases until the orbit begins to become more circular-like causing a decrease in the final kick. Therefore, for each configuration, as we vary $L$, we obtain a maximum in the resultant kick values. An analytic multipolar analysis of encounters for similar configurations can be found in [129]. A recent study by O’Leary, Kocsis and Loeb [135] has found that in dense population environments, there is a non-negligible probability for close flybys or hyperbolic encounters [111]. Most of the cases they considered are those in which after the first passage, the BHs release enough energy to become bound with large initial eccentricity. The hyperbolic encounters we consider in the present work are the extreme case of immediate merger. Nonetheless, kicks with the magnitudes found in the present study could lead to interesting astrophysical consequences.
Chapter 5

Final Mass and Spin of Merged Black Holes and the Golden Black Hole

The spin of the final BH in the coalescence of spinning BHs is determined by the residual angular momentum of the binary. The residual angular momentum consists of the initial orbital angular momentum and spin that the binary is not able to shed via gravitational waves in the process of merging. Unequal-mass, quasi-circular systems with equal magnitude spins aligned or anti-aligned with the orbital angular momentum have been studied extensively with NR, with the cumulative effort resulting in a fit for the final spin [146]:

$$\chi_f = \chi_i \cos \beta \left(1 + s_4 \chi_i \eta + s_5 \eta^2 + t_0 \eta \right) + 2\sqrt{3} \eta + t_2 \eta^2 + t_3 \eta^3,$$

(5.1)

where $\cos \beta = \pm 1$ for aligned or anti-aligned spins, respectively, $(s_4, s_5, t_0, t_2, t_3)$ are fitting coefficients and have values $(-0.129, -0.384, -2.686, -3.454, 2.353)$, the symmetric mass ratio $\eta = m_1 m_2 / (m_1 + m_2)^2$, and $\chi_i = a_i / m_i = |a_1 / m_1| = |a_2 / m_2|$. From the fitting formula, the maximum in the final spin for equal-mass ($\eta = 0.25$), initially extremal spinning BHs is $a/M_h \approx 0.959$. On the other hand, Kesden predicts spins of $a/M_h \approx 0.9988$ for maximally spinning equal-mass mergers [108]. Kesden’s prediction is very close to a maximally spinning BH ($a/M_h = 1$) and rivals the spin of BHs spun up by accretion. In this chapter, we consider equal-mass systems with spins aligned or anti-aligned with the orbital angular momentum. We will not confine the simulations to just the quasi-circular case and study a large family of initial parameters in an effort to find the maximum spin and compare to these reported values.
During quasi-circular inspirals, large amounts of angular momentum is radiated. By considering plunge-dominated encounters, we aim to minimize the amount of angular momentum radiated and thus maximizing the final spin. We wonder if the initial angular momentum of the system is greater than extremal \((J/M^2_{\text{adm}} > 1)\), will the system radiate just enough to get under the Kerr limit \((S_f/M^2_h = a/M_h = 1)\) or will the radiation overshoot the limit, and thus the final spin will be significantly less than \(a/M_h = 1\)? To answer this, we first consider a non-spinning, plunge-dominated configuration with impact angle \(\theta = 26.565^\circ\) in Section 5.1 and vary initial \(J/M^2_{\text{adm}}\). We then extend the study to add aligned or anti-aligned spin configurations and various impact angles from \(\theta = 6^\circ\) to \(\theta = 90^\circ\), again varying the initial \(J/M^2_{\text{adm}}\) for each initial configuration. In this way, we can find a global maximum of the final spin in our two parameter family of \(\{S/M^2, \theta\}\), as presented in Section 5.2.1. This study is the most extensive numerical relativity study of the parameter space of BBH spacetimes, consisting of more than a thousand individual simulations. In Section 5.2.2, we extend the study from direct plunges to more energetic orbits, including multiple encounters, quasi-circular inspirals, and generalizations of Newtonian elliptical orbits. In Section 5.2.3, we analyze the gravitational radiation and trajectories of the orbits of Section 5.2.2.

To classify the simulations performed in this chapter, only three numbers need to be specified due to the initial configuration. All simulations have equal-mass BHs and initial separations, \(d/M = 10\). Unless otherwise noted in the text, both BHs per simulation have spins that are equal in magnitude. Therefore, specifying the total initial spin \((S/M^2)\), the angle between the initial momentum vector and the vector connecting the two BHs (or the impact angle, \(\theta\)), and the total initial angular momentum \((J)\) uniquely identifies the system. The total initial spin in terms of the BHs dimensionless spin parameters, \(a_1/m\) and \(a_2/m\), is

\[
S/M^2 = \frac{1}{(2m)^2}(ma_1 + ma_2) = \frac{1}{4} \left( \frac{a_1}{m} + \frac{a_2}{m} \right),
\]

where \(m\) is the mass of the individual BHs and in this case, \(m = 0.5\). For the cases where the spins are not equal, both dimensionless spin parameters will be used to classify the simulations. The initial total angular momentum is the sum of both the orbital and spin angular momentum:

\[
\frac{J}{M^2} = \frac{L}{M^2} + \frac{S}{M^2} = \frac{P}{M} \frac{d}{M} \sin \theta + \frac{S}{M^2}
\]

where \(P/M\) is the initial momentum of the BHs. The angular momentum \(J/M^2\) is then
normalized with the ADM mass of the system, $M_{\text{adm}}/M$. For a given $S/M^2$ and $\theta$, a series of simulations are performed for increasing $J$. With this classification, the first series of runs studied in Section 5.1 is $S/M^2 = 0.0$ and $\theta = 26.565^\circ$.

The work presented in Section 5.1 has been published in *Physical Review Letters*, 101:061102 [172] and the work in Section 5.2 has been submitted for publication to *Phys. Rev. D: Rapid Communications* [95].

### 5.1 Non-spinning, Equal-Mass Scattering

BBH simulations enable studies of strong non-linear phenomena regardless of traditional gravitational astrophysics consequences. A recent example is the work of Pretorius and Khurana [143] on the self-similar behavior found in the approach to the merger/flyby threshold of BBHs. Similar merger thresholds in BBH encounters or scatterings form the context for this work.

In this section, we consider orbits in which the BHs initially fly past one another, but then fall back to orbit and merge. We focus on the gravitational waveform and the angular momentum radiated from such encounters. Serendipitously, we find significant astrophysical implications, both the existence of a maximum in the final BH spin and of multiple encounter orbits with associated multiple bursts of gravitational radiation. Pretorius and Khurana considered only the first close encounter or “whirl,” and the study did not extend the evolutions to find possible fall-back orbits such as those here considered [143]. While there have been high-order post-Newtonian studies of inspiral, cases studied so far have described relatively smooth inspirals [114]. In addition to the work of Pretorius and Khurana and the work presented in this chapter, these highly eccentric orbits have also been studied by Sperhake *et al.* [162], who considered ultra-relativistic scattering encounters.

All of our orbits are parabolic or hyperbolic encounters. Depending on the merger, the fraction of angular momentum radiated varies significantly ($0.05 \lesssim J_{\text{rad}}/L \lesssim 0.55$ with $L$ the initial orbital angular momentum of the binary). This emission of angular momentum sets an upper limit of $a/M_h \approx 0.823$ for the spin parameter of the final BH; this maximum occurs when $L/M^2_{\text{adm}} \approx 1.001$.

As in previous PSU-GATech BBH studies [97, 98, 99], we use a code based on the BSSN formulation and the moving puncture recipe. The results here were obtained with a $(634 M)^3$ computational domain consisting of 10 refinement levels, with finest resolution of $M/51.6$. We set up non-spinning, equal-mass BHs using Bowen-York initial data as in
Figure 5.1. Top panel, spin of the final BH $a/M_h$ and, bottom panel, angular momentum radiated $J_{rad}/L$ vs. the initial orbital angular momentum $L/M_{adm}^2$.

Section 2.3.1. The mass of each BH is $M/2$, computed from $\sqrt{A_{ah}/16\pi}$ (Equation 3.2) with $A_{ah}$ their apparent horizon area. The data have the BHs on the $x$-axis: BH$_\pm$ is located at $\pm 5 M$ and has linear momentum $\vec{P}_\pm = (\mp P \cos \theta, \pm P \sin \theta, 0)$. We keep the angle constant at $\theta = 26.565^\circ = \tan^{-1}(1/2)$; thus the impact parameter is $\sim 4.47 M$. The total initial orbital angular momentum is given by $\vec{L}/M^2 = 10 (P/M) \sin \theta \hat{z}$. We obtain a one-parameter family of initial data by varying the magnitude of the initial momentum in the range $0.1145 \leq P/M \leq 0.3093$. At the lower limit of the momenta, merger occurs within less than half an orbit of inspiral. We then consider successively higher initial momenta until we find solutions that will clearly require a very long, “infinite” time to merge.

The results are summarized in Figures 5.1 and 5.2. The top panel in Figure 5.1 shows the spin $a/M_h$ of the final BH as a function of the initial orbital angular momentum
Figure 5.2. Top panel, mass of the final BH $M_h/M_{\text{adm}}$, and, bottom panel, energy radiated $E_{\text{rad}}/M_{\text{adm}}$ vs. the initial orbital angular momentum $L/M_{\text{adm}}^2$.

$L/M_{\text{adm}}^2$. The spin and mass of the final BH were computed using the apparent horizon formula, Equations 3.4 and 3.5. The bottom panel of Figure 5.1 displays the fraction of angular momentum radiated ($J_{\text{rad}}/L = 1 - a M_h/L$). Figure 5.2 shows, as a function of $L/M_{\text{adm}}^2$, in the top panel the final mass, $M_h/M_{\text{adm}}$, relative to the total ADM mass and in the bottom panel the fraction of energy radiated $E_{\text{rad}}/M_{\text{adm}} = 1 - M_h/M_{\text{adm}}$. The vertical lines in Figures 5.1 and 5.2 denote the value of $L/M_{\text{adm}}^2$ where $a/M_h$ is maximum. We have also calculated both the radiated angular momentum and energy via the Weyl tensor as in Section 3.2. The results are consistent with those in Figures 5.1 and 5.2. However, the values obtained form $J_{\text{rad}}/L = 1 - a M_h/L$ and $E_{\text{rad}}/M_{\text{adm}} = 1 - M_h/M_{\text{adm}}$ are more accurate because they are not as susceptible to resolution effects as those derived from wave extraction. We have carried out simulations at resolutions of $M/45$, $M/48$, $M/52$ and $M/64$ for ten representative cases in Figures 5.1 and 5.2 to check convergence.
and make error estimates. We found that the results are consistent with the 4th-order accuracy of our code and that the errors in the quantities displayed in these figures are not larger than 3%.

We have selected six encounters that are representative of the different behaviors in our series. These six cases are $L/M^2 = 0.512, 1.208, 1.352, 1.376, 1.382$ and $1.387$ or

**Figure 5.3.** BH tracks of the six representative encounters.
equivalently $L/M^2_{adm} = 0.517, 1.044, 1.120, 1.131, 1.134$ and $1.136$. We will refer to them as encounters Ea, Eb, Ec, Ed, Ee and Ef, respectively. Cases Ed, Ee and Ef correspond to the last three points in Figures 5.1 and 5.2.

For $L/M^2_{adm} < \sim 0.8$, the radiated angular momentum is $J_{rad}/L < \sim 0.15$, so the final BH has $a/M_h$ close to $L/M^2_{adm}$. The evolution is rather simple in these cases: immediate merger, with minimal inspiral. For instance, in case Ea (Figure 5.3), $L/M^2_{adm} = 0.517$, and $J_{rad}/L = 0.05$; thus most of the angular momentum goes into the final BH, $a/M_h = 0.496$. Figure 5.4.Ea shows the corresponding radiated gravitational wave ($M \Re \Psi^2_{4,4}$). All waveforms were extracted at radius $50M$.

As the initial angular momentum increases, the radiated angular momentum also increases, suppressing and limiting the spin of the final BH. Eventually for large enough initial angular momentum, so much angular momentum is radiated that, as seen in Figure 5.1, the final spin reaches a maximum of $a/M_h \approx 0.823$ at $L/M^2_{adm} \approx 1.001$. Figure 5.3.Eb shows the tracks of the BHs in the neighborhood of this maximum. Fig-
Figure 5.5. Real part of the waveforms for the Ed, Ee and Ef encounters.

Figure 5.4. Eb shows the corresponding radiated waveform. For even larger initial angular momentum, the spin of the final BH actually decreases for increasing $L/M_{\text{adm}}^2$. The reason is that the merger is not only preceded by several hangup orbits [55, 143], but also the merger yields a highly distorted BH that radiates copiously as it settles down. Case Ec with $a/M_h \approx 0.68$ and $L/M_{\text{adm}}^2 \approx 1.120$ represents this situation in which almost 50% of the initial angular momentum is radiated (see path in Figure 5.3.Ec and radiated waveform in Figure 5.4.Ec).

A persistent feature of the mergers with $L/M_{\text{adm}}^2 \lesssim 1.045$ is that the separation between the BHs (the coordinate distance between the punctures) decreases monotonically with time (monotonic inspiral). Comparing cases Ea, Eb and Ec in Figure 5.4, there is general qualitative agreement: inspiral-generated gravitational waves with frequency and amplitude increasing in time, followed by essentially fixed-frequency ringdown waves. There is, however, a hint of disappearance of the monotonic spiral in case Ec. The amplitude of the gravitational radiation has a “shoulder” at about time $\sim 110M$. For a
Figure 5.6. BBH coordinate separation for the Ec, Ed, Ee and Ef encounters.

period of time equal to two wave oscillations, the decline of the amplitude ceases and then recommences. The relative orbital separation as a function of time (Figure 5.6.Ec) clearly shows there is a plateau in the separation centered at time \( \sim 50 \, M \), which is absent for cases Ea or Eb. For a brief period of time there is a closely circular phase in which the BHs “want” to fly apart, but just manage to stay at roughly constant separation.

The last three points in Figures 5.1 and 5.2 are the cases labeled Ed, Ee and Ef. They describe orbits without immediate merger but “escape” and recapture; they all
show initial approaches followed by increasing mid-evolution separations of 14 $M$, 25 $M$ and 42 $M$ before the final merger (see Figures 5.3 and 5.6). Because the interaction involves two close approaches, there are two bursts of gravitational radiation, one from the first flyby [179] and the other from the merger (see Figure 5.5). We are currently investigating astrophysical implications of detections of these multiple gravitational bursts and hangups in globular clusters [111].

For the Ef case, there is an approximate hangup, or whirl, with separation $\sim 4 - 5 M$ around time $\sim 950 M$ similar to the shoulder seen in Figure 5.6.Ec around time $\sim 50 M$. This structure shows up in the waveform for this Ef case; there is actually a (lower amplitude) precursor to the radiation burst associated with the merger, a hint that orbits with many repeated bounces are possible. For even slightly (0.1\%) greater initial angular momentum than case Ef, the BHs complete approximately one loop and then escape. This is a possible indication of chaotic behavior (exponential dependence on initial conditions, consult [143]). Repeated bounce orbits would have to be found with initial angular momentum very slightly above that which resulted in Figure 5.3.Ef. As with all critical phenomena, the problem becomes one of careful tuning of the parameters. Note that these interactions of non-spinning BHs produce chaotic orbital dynamics, in contrast to the chaos found in spin evolutions [117, 92].

In this section, we investigated a single series of simulations with spin configuration $S/M^2 = 0.0$ and impact angle $\theta = 26.565^\circ$ by varying the total initial angular momentum $L/M^2_{adm}$. A maximum in the spin can be found in the region between straight plunges and circular-like whirl trajectories. We also found escape and recapture trajectories of up to two encounters, with evidence that more can occur. In the next section, we extend the study to include spins that are aligned or anti-aligned with the initial orbital angular momentum and consider a range of impact angles.

### 5.2 Spinning, Equal-Mass Mergers

An important question that can only be answered with the tools provided by numerical relativity is: what is the final mass and maximum spin of the final BH from generic binary mergers? In Section 5.1, we took the first step towards answering this question. We studied the behavior of a $1-$parameter series of equal-mass, non-spinning BHs in merger or flyby. The adjustable parameter was the magnitude of initial linear momentum $P$ for each of the BHs, or equivalently the initial angular momentum of the system, $\vec{L} = dP \sin \theta \hat{z}$. The main result in Section 5.1 was the specific dependence or transfer
function found that connects the final merged BH spin \( \frac{a}{M_h} \) with the initial \( \frac{L}{M^2_{\text{adm}}} \) (see Figure 5.1, which is repeated in Figure 5.7 in the curve labeled as \( \frac{S}{M^2} = 0.0 \), i.e. vanishing total initial spin). For this case, a maximum final BH spin \( \frac{a}{M_h} \approx 0.823 \) was found at \( \frac{L}{M^2_{\text{adm}}} \approx 1 \).

No previous BH merger simulation has produced final spins close to maximal, for example, \( \frac{a}{M_h} > 0.99 \). We do know from specific examples in work by Campanelli et al. [55] that “hangups” occur, in which the orbital radius decreases only slowly or not at all, and which enable the radiation of substantial angular momentum before the merger. We also found a splash-skip behavior involving what Pretorius and Khurana [143] called whirl orbits for the non-spinning case. In these cases the interacting BHs can approach, then recede to a large distance, then approach again, producing repeated bursts of gravitational radiation. This is clearly an extreme case of “hangup.”

In Section 5.2.1, we extend the study to encounters where at least one of the BHs carries a spin, with the spins parallel or anti-parallel to the orbital angular momentum. The main motivation is to add extra initial angular momentum in order to increase the final BH spin. In addition, we vary the angle \( \theta \), but keep the initial separation as before, \( d = 10 \, M \). We find similar transfer functions to that in the non-spinning case, with the maximum final BH spin depending on the spins of the merging BHs and the scattering angle \( \theta \). Our simulations show that the final BH can reach a maximum spin \( \frac{a}{M_h} \approx 0.992 \) when extrapolated to the merger of BHs that are initially maximally spinning.

In addition, we found an interesting behavior regarding the parameters \( \frac{M_h}{M} \) and \( \frac{a}{M_h} \) of the final BH as the orbital angular momentum is increased. The values for \( \frac{M_h}{M} \) and \( \frac{a}{M_h} \) spiral around the parameters of what we operationally call a golden BH. We have been able to identify the golden BH to be the hole obtained from the merger of a binary in a quasi-circular inspiral with the corresponding spinning BHs. This topic will be discussed in Sections 5.2.2 and 5.2.3.

The computational setup for the simulations presented here is very similar to the one in Section 5.1, the main difference being the added initial spin angular momentum to the colliding BHs and the increase in spatial differencing from fourth order to sixth order. All simulations had 10 levels of refinement, with an outer boundary of \( \sim 320 \, M \). For the runs used to compute the maximum final spin with angle, \( \theta \geq 26.565^\circ \) (\( \sim 200 - 300 \, M \) run times), a resolution of \( M/51.6 \) was used on the finest level, with each subsequent level decreased by a factor of 2. For the maximum final spin runs with \( \theta < 26.565^\circ \) runs (\( \sim 200 - 300 \, M \) run times), a resolution of \( M/103 \) was used. For the longer runs
to compute the golden BH (∼ 500 – 3000 M run times) in Section 5.2.2, a resolution of $M/90$ was used on the finest. Convergence tests were conducted on several representative configurations at resolutions ($M/51, M/64, M/77, M/90, M/103$). We estimate that the errors in the maximum spin results due to the finite differencing are of the order of 2% or less and the errors in the golden BH results are of the order of 1% or less.

**5.2.1 Maximum Final Black Hole Spin**

This section is aimed at addressing the following three questions regarding the maximum spin of the final BH: For spinning BHs, does the maximum occur near the same initial angular momentum as found in Section 5.1? What is the dependence of the maximum residual spin on the value of the initial spins of the merging BHs? How close is the maximum final spin to the Kerr limit? The answer to the first question is “yes”. The maximum for the residual angular momentum occurs near $J/M_{adm}^2 \approx 1$ for all cases considered. This conclusion is apparent from Figure 5.7, where the dependence of the spin of the final BH $a/M_h$ as a function of the initial total (orbital plus spin) angular momentum $J/M_{adm}^2$ at a constant $\theta = 26.565^\circ$ is shown. From top to bottom are the cases $S/M^2 = \{0.4, 0.3, 0.2, 0.1, 0.0, -0.1, -0.2, -0.3, -0.4\}$, respectively, where $S/M^2$ is the total initial spin of the system and is given by Equation 5.2. Each line in the figure consists of approximately ten simulations.

We have looked for but find very little torque-up, suggesting very little spin-orbit coupling. At the same time, for the configurations considered, the final spin as a function of $J$ depends only on the total initial spin, not how it is distributed between the interacting BHs. For instance, the cases $a_{1,2}/m = \{0.4, 0.4\}$ ($S/M^2 = 0.1 + 0.1$), $a_{1,2}/m = \{0.0, 0.8\}$ ($S/M^2 = 0.0 + 0.2$) and $a_{1,2}/m = \{0.6, 0.2\}$ ($S/M^2 = 0.15 + 0.05$), which have the same initial total spin $S/M^2 = 0.2$ but distributed differently between the two BHs, have almost identical dependencies of the final merged BH angular momentum on the initial total angular momentum $J/M_{adm}^2$; see Figure 5.8. We have carried out similar experiments for total $S/M^2 = 0.1$ (with $a_{1,2}/m = \{0.8, -0.4\}$ and $a_{1,2}/m = \{0.2, 0.2\}$) and $S/M^2 = 0$ (with $a_{1,2}/m = \{0.0, 0.0\}$, $a_{1,2}/m = \{0.4, -0.4\}$ and $a_{1,2}/m = \{0.8, -0.8\}$). These results suggest that the initial spin is simply “bundled into” the total $J$ in the evolution. A fraction of $J$ is then deposited into the final BH, so that the final BH spin depends essentially only on the total initial angular momentum.

This result is confounding because a close examination of the orbits shows significant differences between two cases with the same total but different distribution of initial spin. For instance, the case $a_{1,2}/m = \{0.4, 0.4\}$ with symmetrical initial data yields a
Figure 5.7. Spin of the final BH \( a/M_h \) vs. the initial total (orbital plus spin) angular momentum \( J/M_{adm}^2 \) at a constant \( \theta = 26.565^\circ \). From top to bottom are \( S/M^2 = \{0.4, 0.3, 0.2, 0.1, 0.0, -0.1, -0.2, -0.3, -0.4\} \), respectively. Significantly different evolution from the case \( a_{1,2}/m = \{0.0, 0.8\} \). In fact, the \( a_{1,2}/m = \{0.0, 0.8\} \) case produces a kick of \( \sim 175 \) km s\(^{-1}\), and the symmetric case \( a_{1,2}/m = \{0.4, 0.4\} \) does not.

The answers to the second question (“how does the final BH depend on the initial total spin?”) can be found in Figure 5.9 where we show the maximum spin \( a/M_h \) deposited in the final BH versus the initial total spin angular momentum \( S/M^2 \). Each line in this figure consists of several points (5 or more) which are the maximums of the angular momentum transfer functions such as those in Figure 5.7. For example, for \( \theta = 26.565^\circ \), there are nine points in Figure 5.9, one corresponding to the maximum of each line in Figure 5.7. We fit a fourth order polynomial to the points around the maximum in the transfer function to find these maximum values. Each point in Figure 5.9 is the result of about 10-15 simulations, or in other words, to construct Figure 5.9, approximately 400 simulations were done. From top to bottom are \( \theta = \{26.565^\circ, 32^\circ, 45^\circ, 55^\circ, 70^\circ, 80^\circ, 90^\circ\} \), respectively, with the lines for \( \theta = 80^\circ \) and \( 90^\circ \) almost completely overlapped. The dependence of the final spin on the spins of the merging BHs is almost linear for \( \theta \) approaching \( 90^\circ \) but non-trivial for small values of \( \theta \). The small \( \theta \) values correspond to small impact parameters. For these cases, mergers with negative \( S/M^2 \) are direct plunges; very little
Figure 5.8. Spin of the final BH $a/M_h$ vs. the initial total (orbital plus spin) angular momentum $J/M_{adm}^2$ with $S/M^2 = 0.2$ total and $\theta = 26.565^\circ$. Red line for $S/M^2 = 0.0 + 0.2$, blue for $S/M^2 = 0.1 + 0.1$ and pink line for $S/M^2 = 0.15 + 0.5$

Angular momentum is radiated, thus the turn around observed in Figure 5.9.

A possible answer to the third question (“what is the maximum final spin in these mergers?”) can be found by extrapolating the $\theta = \text{constant}$ lines in Figure 5.9 to maximally spinning incident BHs (i.e. to $S/M^2 = 0.5$). Such extrapolation yields a final BH spin $a/M_h \approx 0.98$. This maximum final spin is slightly lower than the prediction for quasi-circular inspirals by Kesden [108] of $a/M_h \approx 0.9988$ but higher than the estimate by Rezzolla [144] of $a/M_h \approx 0.959$. Recently, work by Sperhake et al. [162] has also produced final spins $a/M_h \approx 0.95$ for non-spinning, highly boosted BHs. We believe that these highly boosted BHs address a different regime from the one considered here.

It is important to remember, however, that our study involves a 2-parameter family of simulations in $S/M^2$ and $\theta$. Extrapolation along $\theta = \text{constant}$ as in Figure 5.9 may not be the right path in parameter space to find the maximum final spin. To further investigate this point, we plot in Figure 5.10 the final spin as a function of $\theta$ but now for lines $S/M^2 = \text{constant}$. From bottom to top are the cases $S/M^2 = \{0.0, 0.1, 0.2, 0.3, 0.4\}$. The crosses along the top axis of the figure are the values obtained from the $\theta = \text{constant}$ extrapolation to extremal BHs ($S/M^2 = 0.5$) in Figure 5.9. It is now clear why the values obtained from this extrapolation are very similar to each other: Figure 5.10 shows that
Figure 5.9. Maximum spin deposited in the final BH $a/M_h$ vs. the initial spin angular momentum $S/M^2$ parallel or anti-parallel to $L$. From top to bottom are the cases $\theta = \{26.565^\circ, 32^\circ, 45^\circ, 55^\circ, 70^\circ, 80^\circ, 90^\circ\}$, respectively. Extrapolating to maximal spinning BHs yields the maximum merged BH spin of $a/M_h \approx 0.98$. The final spin for $\theta \geq 30^\circ$ along $S/M^2 = \text{constant}$ lines is roughly constant.

Notice that in Figure 5.10 we have extended the range of simulations to include $\theta \leq 26.565^\circ$. A completely different $\theta$ dependence is found for these smaller angles, whose details are better appreciated in the inset of Figure 5.10. As $\theta$ decreases along each $S/M^2 = \text{constant}$ line, the final spin increases and reaches a maximum. It is now obvious that the maximum spin from the $\theta = \text{constant}$ extrapolation in Figure 5.9 does not yield the global maximum. Instead, a better estimate of the maximum final spin can be found by an extrapolation to extremal BHs using the values of the maximum on each of the $S/M^2 = \text{constant}$ lines in Figure 5.10. The result of this extrapolation yields a maximum final spin $a/M_h \approx 0.992$ at $\theta \approx 15.23^\circ$ and is depicted as a black dot in Figure 5.10. This value is consistent to within error to the value predicted by Kesden [108]. Figure 5.11 has the final mass (both $M_h/M$ and $M_h/M_{\text{adm}}$) that correspond to the maximum final spins in Figure 5.10. These values are in no way the maximum or minimum final mass that can be achieved, but are just the final masses that correspond to the final maximum spins. One thing to note is that the maximums in the lines of constant $S/M^2$ in Figure 5.10 do not correspond to the minimums in the final mass
Figure 5.10. Final maximum spin values for given spin configuration and angle, $\theta$. Each line consists of several series of runs at different impact angles with varying initial angular momentum. The maximum from each series was taken and interpolated to produce the lines. There are five spin configurations $S/M^2 = \{0.0, 0.1, 0.2, 0.3, 0.4\}$, (light blue, pink, blue, black, red). Extrapolating the maxima of these lines to extremal, $S/M^2 = 0.5$, leads to a near extremal BH with $a/M_h \approx 0.992$.

It is important to discuss the top line in Figure 5.10, which corresponds to an initial spin configuration of $S/M^2 = 0.4$. For this line, we do not obtain a “clean” maximum because of an artificial loss of angular momentum like that seen by Marronetti et al. [128]. Marronetti et al. used a fourth order code with reasonable resolutions, and saw a drastic loss of angular momentum for spins greater than $a/M_h \approx 0.75$. With our sixth order code and resolutions of $M/103$ at the finest, this artificial loss of spin still occurs but at spins much closer to maximal in the range of $a/M_h \gtrsim 0.95$. For example, for one simulation near the max of $S/M^2 = 0.4$ and $\theta = 16^\circ$, the final spin decreases from 0.974 at about 60$M$ after merger to 0.964 at about 160$M$ after merger. This is a loss of approximately 1% over a span of 100$M$. An increase in spatial resolution does decrease the artificial loss, but even with high resolution ($M/150$ at the finest) it is still non-negligible. For lower magnitude spins, in general, there is very little change in the spin after merger, with at most some movement in the fourth or fifth decimal place. Since the final mass and
Figure 5.11. Final mass values $M_h/M$ (top) and $M_h/M_{adm}$ (bottom) vs. $\theta$ corresponding to the maximum spin values in Figure 5.10. There are five spin configurations $S = \{0.0, 0.1, 0.2, 0.3, 0.4\} M^2$ (light blue, pink, blue, black, red).

spin are usually very stable over long periods of time after merger, when the extraction of the mass and spin occurs does not affect the results. In general, we choose the mass and spin farthest from merger, when there is no doubt that the remnant BH has settled to a stationary state and all our machinery is valid. For the top line in Figure 5.10, choosing the values far after merger is not valid due to this spurious spin loss. However, choosing the values about $60M$ after merger may be too soon since the BH may not be settled down yet. Since we know that choosing the later values will definitely introduce large errors and kill the precision of the series, we attempt to use the values closer to the merger. At $60M$ after merger, there is still some radiation coming from the ringing BH but the amplitude is very small compared to the maximum amplitude. The values of the
spin taken in this regard are shown in the top line of the Figure 5.10, and interpolation of this line shows a maximum spin of \( a/M_h = 0.977 \) at an angle of \( \theta = 16.48 \). When using the bottom four lines to extrapolate, we project a maximum spin of \( a/M_h = 0.977 \) around \( \theta = 16.4^\circ \) for \( S/M^2 = 0.4 \). These values agree very well, justifying the use of the spin and mass values closer to merger. Further, this means that \( a/M_h = 0.974 \) is the highest simulated BH spin to date. When using all five maximums to extrapolate to initially extremal spinning BHs in Figure 5.10 (as opposed to just the bottom four) the result barely changes, with the maximum final spin \( a/M_h \approx 0.992 \) at \( \theta \approx 15.38^\circ \). Since none of the simulations resulted in a final spin \( a/M_h > 1 \), no naked singularities were observed, and the cosmological censorship conjecture was upheld in all simulations conducted.

### 5.2.2 Golden Black Hole

In addition to studying the maximum possible final spin, we investigated the final state, \( M_h/M \) and \( a/M_h \), as one increases the initial angular momentum \( J/M^2_{adm} \) past the first maximum in the transfer function for \( a/M_h \). In the equal-mass, non-spinning case with \( \theta = 26.565^\circ \) in Section 5.1, as \( J/M^2_{adm} \) increases and the orbital dynamics of the system become more complex, the final spin reaches a minimum and begins to increase again (see Figure 5.1). Due to the rebound separation for the low impact angle cases (for the highest angular momentum in Figure 5.1, a separation of \( r/M = 40 \) is obtained), we consider angles \( \theta \geq 60^\circ \) to investigate this region. The results for the case \( S/M^2 = 0.4 \) with \( (a_{1,2}/m = 0.8) \) and angles \( \theta = \{60^\circ, 80^\circ, 90^\circ\} \) can be found in Figure 5.12. It is interesting that as \( J/M^2_{adm} \) is increased, the pair, \( M_h/M \) and \( a/M_h \), exhibits decaying oscillations around some values, \( M^*_h/M \) and \( a^*/M_h \). After a close examination of the orbits that lead to these results, we concluded that these oscillations are a direct consequence of the binary having to undergo multiple escape and recapture episodes to shed the “excess” of angular momentum that inhibits the merger, see Section 5.2.3 for a discussion of the trajectories for this series of runs. Note also that for a given angle \( \theta \), the amplitude of the oscillations are closely similar between \( a/M_h \) and \( M_h/M \). Furthermore, the frequency of the oscillations is not constant but increases for larger \( J/M^2_{adm} \). The two quantities are \( 90^\circ \) out of phase.

In order to get a better insight into the oscillation and, in particular, to investigate whether the damping of the oscillations continues for larger \( J/M^2_{adm} \), we focused our attention on the case \( S/M^2 = 0.0 \). Vanishing initial spins not only yield shorter merger times but also require lower resolutions, thus reducing the computational cost of the large
number of simulations needed. Figure 5.13 shows $(M_h - M^*_h)/M$ (top) and $(a - a^*)/M_h$ (bottom) versus $J/M^2_{adm}$ for $\theta = 90^\circ$ and non-spinning initial BHs. Crosses are the data from the simulations and solid lines are fits to

\[
\frac{a}{M_h} = \frac{a^*}{M_h} + A \pm e^{\pm B \phi} \sin(\phi) \tag{5.4}
\]

\[
\frac{M_h}{M} = \frac{M^*_h}{M} + D \pm e^{\pm C \phi} \cos(\phi) \tag{5.5}
\]

with $\phi$ a monotonically growing third order polynomial in $J/M^2_{adm}$. The fittings were done as follows. Around $J_*/M^2_{adm} \approx 0.985$ (vertical line in Figure 5.13) the oscillation is almost completely damped out. We have then divided the data into values below and above $J_*/M^2_{adm}$. For those below, we fit a decaying exponential and, similarly, a growing exponential for the data above values $J_*/M^2_{adm}$. The $\pm$ in the constants,
Figure 5.13. Golden oscillations for non-spinning equal-mass BHs with impact angle $\theta = 90^\circ$. The oscillations damp until the quasi-circular region and then begin to increase again. Final mass $M_h/M$ (top) and final spin $a/M_h$ (bottom) vs. initial angular momentum $J/M_{adm}^2$.

$\{A_{\pm}, B_{\pm}, C_{\pm}, D_{\pm}\}$, correspond to the region above (+) and below (−) $J_*/M_{adm}^2$, respectively. For the fitting, we have ignored the points in the neighborhood of $J_*/M_{adm}^2$ since in that region the oscillations are almost completely damped.

An interesting finding is that, modulo a phase shift, $\phi$ is basically the same fitting function (i.e. similar constant coefficients in the third order polynomial in $J/M_{adm}^2$) for the decaying and growing sectors. We also obtain that both the decaying and growing fittings yield the same values of $\{M_h^*/M, a^*/M_h\} \approx \{0.951, 0.685\}$. The only changes are in the constants $\{A_{\pm}, B_{\pm}, C_{\pm}, D_{\pm}\}$. Finally, the exponential envelopes (black lines in Figure 5.13) cross approximately at $J_*/M_{adm}^2$. Finally, we considered non-vanishing total initial spins $S/M^2 = 0.2$ and 0.4. As mentioned before, we only performed runs for the decaying oscillation sector. The fits yielded, respectively, $\{M_h^*/M, a^*/M_h\} \approx$
Figure 5.14. Top: Final spin $a/M_h$ (red) and final mass $M_h/M$ (blue) vs. $J/M^{2}_{adm}$ for $S/M^2 = 0.4$ and $\theta = 90^\circ$ with fits. Bottom: $M_h/M_{adm}$ vs. $J/M^{2}_{adm}$.

{0.936,0.800} and {0.906,0.900} for all angles. We name the BHs with parameters \{$M^*_h/M, a^*/M_h$\} the golden BHs. In Figure 5.15, three different spin configurations, $S/M^2 = \{0.0,0.2,0.4\}$, for $\theta = 90^\circ$ are shown depicting the final spin in the top panel and final mass in the bottom panel. Both the number of oscillations and magnitude of oscillations before quasi-circular decrease with decreasing initial spin.

Figures 5.16 and 5.17 show a three-dimensional and two-dimensional view of the results from Figures 5.12 and 5.13. The vertical line in Figure 5.16 denotes the location of the golden BH. The result is a logarithmic spiral which approaches the golden BH as $J/M^{2}_{adm}$ nears $J^*/M^{2}_{adm}$ from above or below. Where the growing and decaying oscillations meet in the right panel of Figure 5.17, there is a kink resulting in a phase shift of $\Delta\phi \approx 140^\circ$. A similar spiral is found in the $a/M_h$ versus $M_h/M$ plane when the angular momentum $J/M^{2}_{adm}$ is held constant and one plots them instead as a function of
Figure 5.15. Final spin $a/M_h$ (bottom panel) and final mass $M_h/M$ (top panel) for $\theta = 90^\circ$ for three different spin configurations, $S = \{0.0, 0.2, 0.4\} M^2$, (red, blue, pink).

the angle $\theta$. The center of the spiral is again at the golden BH. A different spiral pattern is found when one uses $M_h/M_{adm}$. Instead of having oscillations around a constant value as in $M_h/M$, the oscillations in $M_h/M_{adm}$ are around a linear decay with $J/M_{adm}^2$ (see Figure 5.14); a decay that depends on the angle $\theta$.

A closer look at our simulations reveals the identity of the golden BH as the final BH obtained from the merger of a binary of the corresponding spinning BHs in a quasi-circular inspiral. Figure 5.18 compares the golden values obtained in this chapter to the reported quasi-circular values from two other numerical relativity groups [55, 128]. The red and blue lines are our interpolated golden BH parameters. We see very good agreement with the values in the literature.

From the first studies of binary BH mergers [17, 53, 140], it became apparent that merger waveforms have a simpler structure than was expected. Here we have presented
two more examples of reduction of complexity. One is the invariance of the final BH spin versus the initial total angular momentum (see Figure 5.8) with respect to how the individual spins are distributed between the interacting BHs. The other invariance is the final $\{M_h^*, a^* / M_h\}$ of the golden BH with respect to the angle $\theta$, for a given total initial spin $S/M^2$ (see Figure 5.12). These are explicit reductions of degrees of freedom from the initial data to the final BH. For the golden BH, the final state is confined to a small region of parameter space near the golden BH.
Figure 5.18. Comparison of golden mass and spin values from this study with the reported values of quasi-circular mass and spins in the literature. The red line with crosses and blue line with ×s are the interpolated $M^*_h/M$ and $a^*/M_h$ from the golden BH study, respectively. The asterisks are Campanelli et al.’s spin values [55], and the squares, solid and dotted, are the spin and mass from Marronetti et al. [128].

An important point to note is that even though this equal-mass study covered a very wide portion of parameter space, there was a parameter that we did not vary, the initial coordinate separation $d/M$. We kept this value fixed at $d/M = 10$ and carried out the simulations. However, we did calculate the maximum final spin for initially non-spinning BHs for a separation of $d/M = 20$ and $d/M = 30$. The result is that the maximum in the series both increases, and is shifted over in $b/M = d/M \sin \theta$, with increasing $d/M$. However, to find these maxima for larger initial separation, the initial momentum, $P/M_{adm}$ is becoming very large, and high resolutions are needed to resolve the Lorentz contracted length scale along the direction of motion. Therefore, the error associated with the larger initial separation runs is much higher. Nonetheless, there is evidence that as we increase the initial separation $d/M$ we may be able to get even closer to extremal spinning resultant BHs.
5.2.3 Gravitational Waveforms and Trajectories

As mentioned in the previous section, the oscillations around the golden parameters are explained by the escape and recapture episodes. For a given spin configuration, the orbital behavior can be split into two sections based on the scattering angle $\theta$: one where escape and recapture episodes can occur, and one where they cannot. We will discuss the former region first. For the $S/M^2 = 0.4$ and angles greater than roughly $\theta = 18^\circ$, as the initial angular momentum is increased, the straight plunge orbits begin to become more circular to shed the excess angular momentum so that they can merge. This was discussed for the non-spinning case in Section 5.1 and leads to the first maximum as in Figures 5.1 and 5.7. What happens to the final spin for further increased values of angular momentum is clear from a look at the orbital trajectories and gravitational waveforms. There is a point of merger/no-merger threshold (the homoclinic orbit as discussed in Chapter 6) or the circular-like whirl orbit, where slightly more angular momentum causes the BHs to escape and slightly less causes them to plunge and merge. Around this point, we would expect our first minimum in the oscillation, since a large amount of radiation is radiated in this small radius circular-like orbit. Further increased angular momentum leads to an escape of the BHs which will not become unbound but rather recede to some separation before in-falling again. On second approach, at first there are straight plunges, leading to the build up of another maximum, followed by the circular-like orbit and another minimum, and then another bound escape. This process repeats itself until the angular momentum increases to the critical angular momentum, leading to a pure scatter and unbounded motion: the BHs escaping to infinity. It is through these multiple encounters that we observe oscillations around the golden parameters. Figure 5.19 shows the relative coordinate separation of the BHs for the case $S/M^2 = 0.4$ and $\theta = 90^\circ$ versus orbital phase for the extrema of Figure 5.14. The black lines correspond to the maxima and the blue lines to the minima. The ordering of extrema runs from left to right. The first black line closest to the left corresponds to the first maximum which is not shown in Figure 5.14 while the other four black lines correspond to the next four maxima shown. Note that each subsequent maximum or minimum occurs after another escape and recapture episode. All maxima seem to plunge from slightly below $r/M = 4$, while all minima plunge from slightly above but with a period of slow down around $r/M = 2$.

Figure 5.20 shows the relative separation versus phase diagrams for several simulations done in the case of $S/M^2 = 0.0$ and $\theta = 90^\circ$. From this figure, we can see the effects of increasing the angular momentum, and how it causes the escape and recap-
ture episodes. As angular momentum is increased, the merger time and phase increases monotonically. The trajectories as a whole form a continuous deformation as the initial angular momentum is increased, with the humps forming from the more circular-like parts of slightly lower angular momentum orbits. Figure 5.21 shows the orbits of a few simulations in the $S/M^2 = 0.4$ and $\theta = 60^\circ$ where we can see the complicated orbital dynamics and repeated escapes and recaptures.

The escape and recapture episodes also explain why the oscillations damp until a certain point and begin to regrow. By looking at the trajectories for the case $S/M^2 = 0.0$ and $\theta = 90^\circ$ in Figure 5.20, this growth and decay can be understood. Since all the momentum is initially in the tangential direction, the initial point will either be an apobothron (bothron originating from the Greek bothrus, meaning pit [78]) when below quasi-circular $J/M_{adm}^2$, or peribothron when above quasi-circular. Approaching the quasi-circular orbit (red line) from below, two things occur; the number of escape and recapture episodes increases, and the amplitude of the escape and recapture episodes decreases, or in other words, the eccentricity decreases. The quasi-circular case has zero eccentricity, therefore there should be no ‘wiggles’ in the orbit, and the relative separation
should be a monotonically decreasing function with time (see Figure 5.25 for example). Above quasi-circular, the amplitude of the oscillation begins to grow, eccentricity again increases, and the oscillations in the final mass and spin begin to grow. Therefore, the amplitude of the oscillations around the golden parameter are related to the orbital eccentricity. For cases with \( \theta \neq 90^\circ \), there are components of the initial momentum in both the \( x \) and \( y \) directions, and therefore the BHs are not at peribothron or apobothron, and can never reach a quasi-circular case by construction. For this case, the oscillations decay to some point and then begin to grow again without ever completely damping, as shown in Figure 5.22.

In the region around \( J_\ast/M^2_{adm} \approx 0.985 \) in Figure 5.13 there is a small plateau with final spin \( a/M_b \approx 0.685 \) and mass \( M_b/M \approx 0.951 \). It is in this range that our initial orbital eccentricity can be shed fully before merger through radiation reaction, leading to the same final parameters. However, at this initial separation (\( d/M = 10 \)), any other initial angular momentum case does not have time to fully shed its eccentricity. This can be relevant to gravitational wave detection, depending on how much residual eccentricity is left when the waveform enters the detector’s bandwidth [42].

Further, there is a correspondence between different cases that give the same final
Figure 5.21. Trajectories for four cases in the series $S/M^2 = 0.4$ and $\theta = 60^\circ$. Top row from left, $J/M_{\text{adm}}^2 = 1.113, 1.225$. Bottom row from left, $J/M_{\text{adm}}^2 = 1.267, 1.313$.

parameters. For example, take the spin case $S/M^2 = 0.4$ for angles $\theta = 60^\circ$ and $\theta = 90^\circ$. In Figure 5.12, there are several points where the oscillations for these two angles intersect. Choosing one point of intersection (that intersects in both the mass and spin curves simultaneously) as best as possible with the simulations conducted, we can compare the trajectories and waveforms of both cases. One such case is $\{\theta, J/M_{\text{adm}}^2\} = \{60^\circ, 1.318\}$ and $\{90^\circ, 1.200\}$. It is clear from Figure 5.23 that the $\theta = 60^\circ$ is a piece of some $\theta = 90^\circ$ case with a different initial apobothron but same spin configuration. The $\theta = 90^\circ$ line corresponds to a segment of the $\theta = 60^\circ$ trajectory, and both lead to approximately the same final mass and spin; for $60^\circ$, $\{M_h/M, a/M_h\} = \{0.9052, 0.8959\}$, and for $90^\circ$, $\{M_h/M, a/M_h\} = \{0.9048, 0.8962\}$. The slight difference in the final parameters can be attributed to the small differences in the waveforms and trajectories. Even though two distinct initial data sets lead to the same final configuration, one set corresponds to the
other at an earlier point on its path. This suggests that there is only one path to a final BH for a given initial spin configuration.

Even though the separation between the two BHs is coordinate-dependent, we know that this escape and recapture behavior is physical because we observe its signature in the gravitational waveform. For each bounce in the trajectory, we observe a small burst of radiation for when the BHs are at their closest, just like in Figure 5.5 for the non-spinning, $\theta = 26.565^\circ$ case. Unlike that figure, however, there are multiple bounces, and thus multiple bursts of radiation. Figure 5.24 shows the waveforms for trajectories shown in Figure 5.21 ($S/M^2 = 0.4$ and $\theta = 60^\circ$). Figure 5.25 shows the waveform and trajectory for the quasi-circular case in the $S/M^2 = 0.0$ and $\theta = 90^\circ$ series.

One of the other questions we investigated was whether the oscillations are a non-linear phenomenon. It was suggested in a private communication with Kesden, Chen,
Figure 5.23. Waveforms and trajectories for two cases with spin $S/M^2 = 0.4$. The red lines are $\theta = 60^\circ$ and $J/M_{adm}^2 = 1.318$ and the blue lines are $\theta = 90^\circ$ and $J/M_{adm}^2 = 1.200$. The blue lines have been shifted so that merger times are approximately equal.

and Sperhake of the California Institute of Technology [109] that the oscillations may be the result of a continuous sequence of simulations and may be reproducible with PN approximations. To investigate this, we used an PN evolution code based on the 3PN Hamiltonian and 3.5PN radiation reaction term, see Appendix B. For the $S/M^2 = 0.0$ and $\theta = 90^\circ$, the same initial parameters of the NR simulations were used as the initial state of the PN evolution, and the system is evolved until a separation of $r = 3M$ is reached. At this point, the final mass and spin of the BH are estimated using the Hamiltonian and orbital angular momentum of the PN system. From this, the oscillations are reproduced qualitatively but not quantitatively using PN approximations, producing similar oscillations, but around different golden values, with different frequency oscillations, and no phase shift between mass and spin. However, this shows that the oscillations
Figure 5.24. Waveforms for the four cases in the $S/M^2 = 0.4$ and $\theta = 60^\circ$ series displayed in Figure 5.21. All waveforms were extracted at $r = 50M$. 
are not a non-linear phenomenon, but that full GR is required to get the details of the oscillations correct.

The oscillations around the golden parameters and the exponential decay/growth can be explained by the escape and recapture episodes and the amount of eccentricity initially in the system. The signature of this behavior is present in the gravitational waveforms. The oscillations are not a non-linear effect and can be qualitatively reproduced using PN approximations. However, there are still several mysteries about the oscillations. For one, why do they occur around the quasi-circular parameters? Further, why does the mass oscillate as well, and why are the oscillations $\sim 90^\circ$ out of phase? We are currently investigating these questions.

As a final note, for angles below a certain critical value, no escape and recapture episodes can occur. In our above example case $S/M^2 = 0$, this cut-off was roughly $\theta_* = 18^\circ$. For angles $< \theta_*$, the advancing BHs form a common horizon on first approach, and therefore no matter how much angular momentum is pumped into the initial configuration, the BHs cannot escape. It is in this regime that we were able to find the global maximum for each spin case, leading to the extrapolated values of $a/M_h \approx 0.992$. 

**Figure 5.25.** Waveform and trajectory for the quasi-circular configuration $J/M_{\text{adm}}^2 = 0.981$ for the series $S/M^2 = 0.0$ and $\theta = 90^\circ$. The waveform was extracted at $r = 50M$. 

Chapter 6

Zoom-Whirl Orbits

The two-body problem in Newtonian gravity has a closed form solution, and each trajectory can be described by a different conic section. Unbound motion is described by hyperbolas with eccentricity $e > 1$, and parabolas with eccentricity $e = 1$. In general, bound motion is described by ellipses with eccentricity $0 \leq e < 1$, with the circle being the special case of eccentricity $e = 0$. Bound Newtonian motion of a two-body system is always closed, that is the apocentre is constant and always occurs at the same angle $\phi$. It is not until other factors are taken into account, like perturbations from other planets in the solar system, that the orbits can precess. Using Mercury as an example, a large portion of the precession of its perihelion can be accounted for due to the pull of Jupiter and the other planets. Even so, there is still a small amount that is unaccounted (43$''$). Some of the earliest evidence in support of General Relativity is the prediction of exactly 43$''$ contribution to the precession.

In GR, the conic sectional trajectories of the two-body problem are lost, and a closed form solution is not known. However, one thing is clear: even for just two-bodies, precession is a general feature. The best way to gain an understanding of precession is to use an approximation to GR, called the post-Newtonian (PN) approximation. The two-body problem can be solved numerically with the 3PN Taylor Expanded conservative Hamiltonian with spin-orbit coupling and Hamilton’s Equations of Motion (see Appendix B). More interestingly, a form of extreme precession is found, called zoom-whirl precession. The name comes from a description of the dynamics; whirls referring to the nearly circular orbits of at least $2\pi$ each around a small radius, before zooming out to large separations in elliptical leaves. The zoom-whirl dynamics have been studied in the extreme mass ratio inspirals [21, 82] and as aforementioned, in the conservative PN approximations to the two-body problem [87, 118]. A special case of zoom-whirl
behavior has been found in full numerical relativity equal-mass, non-spinning BBH simulations [143] where the initial parameters were fine-tuned and the separatrix was found [87, 120, 137]. The separatrix refers to the orbit between bound motion or plunge and merger, where the number of whirls is infinite. We have also seen zoom-whirl behavior in this dissertation for equal-mass spinning BBH spacetimes in Chapter 5 which consisted of mainly multiple zooms (see Figure 5.20).

Astrophysically, highly eccentric orbits like those needed for zoom-whirl dynamics can be found in dense galactic nuclei [135] or globular clusters [111, 173]. Therefore, we ask: do physically realistic black hole binaries show zoom-whirl behavior? If so, are the waveforms generated different from quasi-circular waveforms such that they could be detected by LIGO? Will zoom-whirl behavior be able to survive the dissipation caused by gravitational radiation? Do we have to finely tune the initial parameters to find the zoom-whirl behavior, or does it occur over a broad range of parameters? In a collaboration with Janna Levin of Columbia University, these questions are answered by using an analytic approximation to get an idea of where the zoom-whirl behavior is expected, and then by running full numerical simulations with these initial parameters. A full scan of initial parameters is not presently possible at the current time due to the computational cost of these simulations. Small masses need large resolutions which directly affects the size of the time step. The runs with multiple zooms are very long, taking several days, and even weeks to complete. Thus, initially we limit the study to one fiducial BBH setup to investigate the zoom-whirl behavior.

For a given angular momentum, zoom-whirl behavior has been quantified [119] and can be described by a single number that specifies the precession of the orbit per radial cycle from apocentre to apocentre. The amount of precession is quantified by

$$\Delta \phi_{\text{precess}} = 2\pi q \quad \text{where} \quad q = w + \frac{v}{z}.$$  \hspace{1cm} (6.1)

The integer, $z$, is the number of zooms, or in other words, the number of leaves in the orbital structure, for example, a $z$-leaf clover. The integer, $w$, is the number of whirls, or the nearly circular orbits close to the pericentre, per leaf. The integer, $v$, is the order in which the leaves are traced out. The clearest way to explain the quantities, $w$, $z$, and $v$, is to look at a few examples with the trajectory to the first apocentre distinguished from the full behavior as in Levin and Grossman [118]. Figures 6.1–6.4 all show zoom-whirl behavior and were generated using a conservative PN evolution code detailed in Appendix B. The top left panel of Figure 6.1 shows an orbit with $q = 1/3$, and the bottom left panel shows an orbit with $q = 2/3$. Both look very similar in
Figure 6.1. Zoom-whirl behavior characterized by $q = \frac{1}{3}$ (top left), $q = \frac{2}{3}$ (top right), $q = \frac{2}{5}$ (bottom left) and $q = 1\frac{1}{3}$ (bottom right). The blue line indicates how the leaves are traced out. In the top left panel, the closest leaf to the initial apocentre is traced first, there are three leaves, and no whirls, therefore $w = 0, v = 1, z = 3$. In the bottom left panel, the second of three leaves is traced first with no whirls, so $w = 0, v = 2, z = 3$. In the top right panel, the second leaf of five is traced first with no whirls, therefore $w = 0, v = 2, z = 5$. In the bottom right panel there is a single whirl before tracing out the first of three leaves, therefore $w = 1, v = 1, z = 3$. Initial parameters for all four cases were $r = 30M$, $a_1/m_1 = a_2/m_2 = 0.5$ aligned with $L$, and $m_1/m_2 = 2$. The initial angular momentum for the given $q$ values is $L/\mu M = 2.089500, 2.078800, 2.065000, 2.061777$ for increasing $q$.

structure, but the ordering of the leaves is different. For $q = 1/3$, the $\Delta \phi_{precess} = 2\pi/3$, meaning between successive apocentres the total precession is $2\pi/3$. Therefore, the order of apocentres is $0 \rightarrow 1 \rightarrow 2 \rightarrow 0$ and so on, with apocentre number 1 being the first leaf closest to the initial apocentre as we increase $\phi$ counterclockwise from the $+x$ axis. For $q = 2/3$, the amount of precession is $\Delta \phi_{precess} = 4\pi/3$, so the order of leaves is
Figure 6.2. Top Left Panel: $q = 1/4$ orbit for same setup as in Figure 6.1 with $L/\mu M = 2.111000$. Top Right Panel: An orbit very close to $q = 1/4$ with $L/\mu M = 2.113000$. The orbit appears to be the precession of the 4-leaf clover in the left panel. Bottom Panel: More structure of the precessing 4-leaf clover is shown.

0 $\rightarrow$ 2 $\rightarrow$ 1 $\rightarrow$ 0. Thus, despite the same number of zooms, the orbit’s structure is definitely different. The top right panel of Figure 6.1 shows a zoom-whirl with $q = 2/5$ with a precession $\Delta \phi_{\text{precess}} = 4\pi/5$, that is 0 whirls, 5 leaves, and the second leaf is traced first. The bottom right panel shows a zoom-whirl orbit with 1 whirl and 3 zooms and therefore has precession $\Delta \phi_{\text{precess}} = 8\pi/3$. A closed Newtonian ellipse corresponds to $q = 0$, precession of Mercury to $q \sim 10^{-7}$, and zoom-whirl behavior for $q > 1$. Any generic orbit would have an irrational $q$, but can be approximated by a nearby rational $q$ (see Figure 6.2). Each individual member of the two-body system will trace out the same shape orbit, as in Figure 6.3. Zoom-whirl behavior can be amplified by increased mass ratios, or increased spin. Larger mass ratios lead to more time spent in orbit (for
Figure 6.3. Left panel: $q = 3/8$ orbit for same setup as in Figure 6.1 with $L/\mu M = 2.081870$. Right panel: The same orbit but showing the motion of the two individuals BHs in the system.

fixed initial starting separation). Spin has a similar effect where spin-orbit coupling produces a ‘repulsive force’ between the BHs when spin and angular momentum are aligned, resulting in longer merger times. Therefore, we would like to maximize the spin and mass ratio as high as realistically possible for numerical simulations presently.

The work presented in this chapter has been published in Physical Review Letters, 103:131101 [96].

6.1 Setup

The course of action to study the zoom-whirl behavior becomes: 1) choose a mass ratio, spin configuration, and initial apobothron, 2) use an effective potential method from the PN approximation to find the range of angular momentum, 3) perform full NR runs around this range. At the turning points of the motion, the Hamiltonian can be used as an effective potential [87, 119]. Figure 6.4 shows the effective potential for two values of $L/\mu M$ and the resulting orbital motion for apobothron $r/M = 30$. In the top row, it is clear that there are two extrema, a stable circular orbit around $r = 13M$, and a marginally bound ($V_{\text{eff}}/\mu = 0$) unstable circular orbit around $r = 4.5M$. The value of the angular momentum that gives this innermost bound circular orbit (ibco) is denoted as $L_{\text{ibco}}$ and is the highest value of the range of angular momentum to search for zoom-whirl behavior. A particle at rest at infinity would approach and whirl an infinite number of times at the ibco. This orbit is known as the separatrix and has $q = \infty$ (infinite whirls) and as the homoclinic orbit of eccentricity 1. As angular momentum is decreased from $L_{\text{ibco}}$,
Figure 6.4. The 3PN effective potential for mass ratio $m_2/m_1 = 1/3$ and spin amplitudes of $-0.3$. Both spins are anti-aligned with the orbital angular momentum. The top is roughly the angular momentum of the ibco, $L_{ibco}/\mu M \sim 4.4$. The straight line corresponds to the orbit $r_a = 30M$. The bottom corresponds to the value of $L/\mu M \sim 4.1$ for which the orbit starting at $r_a = 30M$ becomes the separatrix.

The unstable circular orbit decreases as well and thus, there is a new separatrix. The bottom row of Figure 6.4 shows the effective potential for a lower angular momentum, and we can see that a separatrix occurs now for an initial apobothron of $r = 30M$. Since the unstable orbit will continue to decrease as angular momentum decreases, for an initial separation of $r = 30M$, lower initial angular momentum will lead to an orbit that would pass over the potential and continue to $r = 0M$. Therefore, this value of the angular momentum would be the lower limit on the angular momentum to search for zoom-whirl behavior, and is denoted $L_{\text{min}}$. In general, however, zoom-whirl behavior can be expected until the the unstable circular orbit and the stable circular orbit merge at the innermost stable circular orbit (isco) in the effective potential picture, with the
angular momentum denoted by $L_{isco}$.

We choose a mass ratio of $m_2/m_1 = 1/3$, spins anti-aligned with the angular momentum and with equal magnitudes $a_1/m_1 = a_2/m_2 = 0.3$, and an initial apobothron $r_a = 30M$. The range from the PN effective potential for this configuration is shown in Figure 6.4 with $4.1 < L/\mu M < 4.4$. To start, the lower limit $L = 4.1\mu M$ is simulated using the full NR treatment and is found to have multiple zooms and no whirls, and thus, the homoclinic orbit should occur for $L < 4.1\mu M$. Therefore, we adjust our search range to be $3.9 < L/\mu M < 4.1$ for the NR simulations.

There are a few reasons why the range predicted by PN may not be what we observe with NR. For one, the angular momentum is not constant throughout a full NR run due to the release of gravitational radiation. If angular momentum were constant, $q$ would decrease monotonically with decreasing energy (or equivalently initial apobothron). However, with the release of gravitational radiation, carrying away both angular momentum and energy, the evolution of $q$ is not so straightforward. So as angular momentum decreases, the effective potential decreases, and as energy decreases the apobothron decreases, leaving $q$ to change as well with time. The second reason is that the PN approximation is just that, an approximation. It is not valid in the strong field regime, when the separation is small. Lastly, spin-spin coupling terms were not included in the conservative dynamics because with them a clean effective potential can not be rendered [87, 119].

The runs performed were simulated using the PSU-GATech MayaKranc code that uses the same computational infrastructure and methodology as in previous studies [97, 98], and those discussed in Chapter 2, namely a BSSN code with moving puncture gauge conditions using the Kranc code generator. The black-hole encounters are initiated with Bowen-York initial data. The black holes are located on the $x$-axis: $bh_\pm$ are located at $x_+ = 7.5M$ and $x_- = -22.5M$ where $m_+ = 3M/4$ and $m_- = M/4$. The spatial finite differencing is sixth order. We used eleven levels of refinement with Carpet. The finest resolution is $M/143$ and the outer boundary is at $287M$.

### 6.2 Results

In general, we find zoom-whirl behavior very close to the PN predicted range. Three representative NR cases are presented in Figures 6.5 and 6.6. Figure 6.5 shows the orbits for three values of $L/\mu M$ and the generated waveform. $L = 4.1\mu M$ is shown in the top row, exhibiting what looks like a diminishing two leaf clover, so $q$ is roughly $1/2$. Note
Figure 6.5. Waveforms and relative trajectories of the three cases shown in Figure 6.6. Top left panel: $L/\mu M = 4.10$. The orbit rapidly moves through zoom-whirl cycles precessing by $> \pi$ ($q \sim 1/2$) between apobothrons. Middle left panel: $L/\mu M = 3.95$. The orbit precesses by nearly $> 2\pi$ ($q \sim 1$) in the first radial cycle before merging. Bottom left panel: $L/\mu M = 3.915$. The orbit is very nearly homoclinic, precessing by $\sim 4\pi$ ($q \sim 2$) around the unstable circular orbit before merging. Right Column: The gravitational waveforms for each case in the left column are shown. Each distinctly shows the zoom-whirl behavior, with short bursts for each zoom and long chirps for whirls. Waveforms were extracted at an extraction radius of 60$M$. 
Figure 6.6. The relative orbital separation is plotted vs. the orbital phase for the series of $L/\mu M$ in Figure 6.5. As $L/\mu M$ increases the BHs go through multiple orbits before plunge. Cases shown $L/\mu M = (3.915, 3.950, 4.100)$ (red, blue, pink).

that $q$ is changing rapidly during the orbit and therefore can only be estimated roughly. The second row, $L = 3.95\mu M$, exhibits approximately one whirl so $q \sim 1$. The bottom row, $L = 3.915\mu M$, has approximately two whirls ($q \sim 2$) before falling and merging and is very close to the separatrix. All of the mergers in Figure 6.5 merge by rolling over the effective potential through a whirl and not through the isco. The circular like orbits depicted are not the same as a full circularization of the orbit.

The second column in Figure 6.5 shows the gravitational waveform generated by the zoom-whirl behavior. As the BHs zoom around each other, like in the top right panel, a relatively low magnitude, short burst of gravitational radiation is released. There is one burst for each close encounter. We see a relatively constant magnitude release of gravitational radiation as the BHs whirl around each other at constant separation for $\sim 150M$, as in the bottom right panel. These waveforms are definitely distinct from quasi-circular waveforms (compare Figure 5.25 in Chapter 5) and can therefore be detected in the data stream using algorithms for burst searches or matched filtering techniques.

Figure 6.6 shows the relative separation of the BHs versus the accumulated phase normalized with $2\pi$ for the same three cases of $L/\mu M$ in Figure 6.5. As $L/\mu M$ decreases, the merger time rapidly decreases as well. The PN predicted value for the isco is $r_{isco} \sim$
Figure 6.7. Comparison of the quasi-circular system (blue) and the two whirl system (red). The top panel shows the relative orbital separation vs. time, and the bottom panel shows the 2,2 component of $|\Psi_4|$. However, it is clear from this figure that all of the systems begin to plunge around $r \sim 5M$, which is the peribothron for the whirls predicted in Figure 6.4. Therefore, it is clear from Figure 6.6 that the BHs merge through a whirl phase and not through the isco. The top pink line corresponding to $L = 4.1 \mu M$ shows three zooms before merging. The bottom red line shows approximately $4\pi$ rotation around the unstable circle orbit and is almost homoclinic. To further illustrate the merge through the whirl, Figure 6.7 compares a quasi-circular orbit with the $L = 3.915 \mu M$ system. In the top panel, the two runs are shifted so that their merger times line up, showing distinctly different trajectories for the last few orbits before merger. The bottom panel shows the magnitude of the 2,2 component to $\Psi_4$. Notice the increased amount of radiation from the whirl phase. This suggests that the final mass and spin of the remnant BH will be less than the quasi-circular case. A rough estimate of the mass and spin from
energy and angular momentum conservation confirms this. We expect to observe the oscillations around the quasi-circular *golden* values as in Chapter 5. However, we do not have enough simulations to map the oscillations, but do plan on returning to this topic in the future.

We find that in general, zoom-whirl behavior can survive the dissipatory effects of the full NR treatment. Further, the zoom-whirl behavior is not confined to a small set of initial parameters and can be found broadly. However, to find very high-$q$ zoom-whirl behavior (many whirls) we would have to get arbitrarily close to the homoclinic orbit, which does indeed require fine-tuning. The gravitational radiation from these encounters are distinct showing small bursts for zooms, and larger glitches for whirls. From the PN approximation, there are three factors that can increase the intensity of zoom-whirl orbits, a higher mass ratio, larger spin magnitudes, and larger initial apobothron. In the future, we plan to revisit the zoom-whirl behavior by pushing for more extreme (numerically) values of these factors, extracting a measure of $\dot{q}$, and looking for the oscillations in final spin and mass around the quasi-circular values.
Chapter 7

Summary and Conclusions

In the past few years, numerous studies have been completed on binary black hole coalescence thanks to major breakthroughs in numerical relativity. This dissertation complements these studies, investigating generic BBH mergers over a very large family of parameters.

In Chapter 4, we studied a single scattering configuration with interest in the final kick of the remnant BH. The premise for this research was based on the fact that the majority of the kick was generated during the plunge, and therefore plunge-dominated systems could produce very high kicks. All simulations done for this study were equal-mass, had BHs situated on the $x$-axis separated by $d/M = 10$, and given initial momentum, $\vec{P}/M$ at an angle of $\theta = 26.565^\circ$ with respect to $\vec{d}/M$. Configuring the initial spins to be equal-magnitude but oppositely aligned in the orbital plane, we found sinusoidal behavior of the final kick dependent upon the angle between the spin and momentum and a linear dependence of the final kick on the magnitudes of the initial spins. Both of these characteristics are the same as the kicks generated from quasi-circular configurations. However, the plunge-dominated encounters lead to an enhancement of the final kick, with kicks as high as 10,000 km s$^{-1}$ for the configuration studied; about $2.5\times$ the highest kick proposed for quasi-circular BBH mergers and the highest kick simulated to date.

In Chapter 5, we carried out the most comprehensive study of the parameter space of generic equal-mass BBH mergers, with interest focused on the final mass and spin of the remnant BH. By considering plunge-dominated systems, we hoped to minimize the amount of gravitational radiation emitted, and achieve final BH spins close to the Kerr limit. To investigate this, we considered systems of BHs with initial momentum $\vec{P}/M$ at angle $\theta$ with respect to the $\vec{d}/M$. The BHs were separated by $d/M = 10$. The BBH system had spin $S/M^2$ initially, aligned with the orbital angular momentum.
We then chose combinations of $\theta$ and $S/M^2$ and varied the initial momentum, with $\theta$ ranging from $6^\circ$ to $90^\circ$, and $S/M^2$ from $-0.4$ to $0.4$. For each given angle and spin configuration, as $J/M^2_{adm}$ is increased, a maximum in the final spin is obtained. Plotting these maxima versus initial $\theta$, for lines of constant $S/M^2$, we can extrapolate to initially extremal spinning BHs and find the maximum spin of $a/M_h \approx 0.992$ at $\theta \approx 15.23^\circ$, consistent with the maximum spin predicted by Kesden [108]. Further increasing the initial angular momentum past the first maximum in the spin results in zoom-whirl behavior. This zoom-whirl behavior causes subsequent extrema for both the final mass and spin, leading to oscillations around some golden values. Coincidentally, these golden values turn out to be the final mass and spin from the quasi-circular merger with the same spin configuration. The oscillations occur for all initial angles and spin configurations and occur in two parts, exponential decay and growth, with a phase shift occurring between the two regions. The mass oscillation is out of phase with the spin by $\approx 90^\circ$. There are a lot of questions remaining about these oscillations. For instance, why do they occur around the quasi-circular values, and why is the mass and spin approximately $90^\circ$ out of phase? Is the phase shift between the exponential decay and growth sectors physical or due to numerics? We are currently investigating answers to these questions.

In Chapter 6, we studied zoom-whirl orbits using post-Newtonian approximations and numerical relativity in a collaboration with Dr. Janna Levin of Columbia University. Conservative PN approximations predict zoom-whirl behavior for a wide range of initial angular momentum. However, it was not obviously clear that this zoom-whirl behavior could survive the dissipatory effects of full General Relativity. We chose a fiducial initial configuration: mass ratio $m_2/m_1 = 1/3$ with spins $a_1/m_1 = a_2/m_2 = 0.3$ anti-aligned with the angular momentum. The BHs started at an apobothron (or in terms of impact angles, $\theta = 90^\circ$) with coordinate separation of $d/M = 30$. Like the previous studies, the initial angular momentum was varied by changing the initial momentum and keeping the coordinate separation fixed. We found that, in general, the zoom-whirl behavior does indeed survive and is not confined to a small range of initial angular momentum. The zoom-whirl episodes are clearly distinguishable in the gravitational waveform: with short bursts of radiation for each close encounter, and long, constant magnitude precursors to the plunge for the whirl.
7.1 Towards the Future

Many numerical relativity groups are moving towards non-vacuum BBH studies. Indeed, this is the direction that the PSU-GATech group is moving, and what I will be working on in the near future. However, there are a lot of open-ended questions from the studies presented in this dissertation that can be addressed with vacuum simulations. Further, there are some extensions to these studies that can be performed.

In Chapter 5, we carried out an extensive study of the final mass and spin of the remnant BH. In contrast, we chose only one configuration ($\theta = 26.565^\circ$) for the kicks study in Chapter 4. Ideally, we would like to perform a study of the same magnitude for the final kick. Further, we would like to take advantage of the higher accuracy offered by local calculations of the kick so the implementation of a horizon calculation of the momentum is needed. In conducting this study, we would like to find the maximum final kick that can be achieved and to determine whether there are oscillations around some golden value. We expect the oscillations to occur because we will again observe zoom-whirl behavior. There is evidence for this in Figure 4.3. In the first figure, we obtain a maximum in the final kick just like in the final spin in Figure 5.1. The decrease is due to the same reason as for the decrease in the spin: a more circular-like orbit develops for increasing angular momentum. In Figure 4.5, there is an anti-kick, which developed due to the period of orbital hangup, producing beamed gravitational radiation oriented opposite to the merger and ringdown radiation. Expected for larger initial angular momentum is the development of multiple encounter orbits and zoom-whirl behavior, and therefore, increased likelihood for oscillations in the final kick. Further, we could also study the final mass and spin simultaneously with the kick and see if there is any relationship between them.

All studies presented in this dissertation, besides the zoom-whirl study in Chapter 6, were of equal-mass BBH systems and started with a separation of $d/M = 10$. Therefore, similar studies to the ones presented here for kicks and spin with varying initial separation and unequal-mass systems would exhaust the remaining parameters. If the trends of equations for the projected kicks and spins (Equations 4.1 and 5.1) for quasi-circular systems persist for generic BBH mergers, it may be possible to get even closer to extremal spins and higher kick magnitudes than what was found for the equal-mass study.

Zoom-whirl behavior can be amplified by an increase in the mass ratio, spin magnitudes, and initial apobothron for a given angular momentum. We would like to push the bounds of numerical relativity to more extreme mass ratios than the $m_2/m_1 = 1/3$ considered in this dissertation, and find a way to quantify the change in the zoom-whirl
parameter, $\dot{q}$. We expect to observe the golden oscillations in the final mass and spin from these zoom-whirl mergers.

With the advent of hydrodynamical NR codes, a way to quantify the difference between vacuum waveforms and hydro waveforms is needed. We can achieve this by using a technique that has been employed for use in the detection of gravitational waves, a technique called *matched filtering* (see Appendix C). This technique has been used already for NR studies by Bode *et al.* for waveforms generated by different initial data [34] and by Vaishnav *et al.* to compare waveforms with various resolutions and initial angular momentum [168]. For hydrodynamical studies, we could use the matched filtering techniques to determine how the presence of matter affects the gravitational radiation of a BBH system. Further, it could be used to quantify the amount of matter needed to drastically alter the waveforms. Matched filtering is no doubt a vital tool to have implemented.

Generic BBH mergers lead to interesting structure in the final mass, spin, and kick of the remnant spacetime. Since the first successful BBH simulations, a tremendous amount of knowledge about gravitational radiation, the mathematical properties of Einstein’s Equation, and BBH spacetimes has been uncovered. Much has been accomplished in this dissertation, but there is much left to uncover and many unanswered questions to address. The machinery is in place, and with enough (computer)time and effort, these mysteries will be solved.
Appendix A

Notation and Conventions

Throughout this dissertation, the metric convention of Misner, Thorne, and Wheeler [130] is used, where the spacetime metric $g_{\mu\nu}$ has signature $(-, +, +, +)$. Greek indices are used for four-dimensional quantities and Latin indices are used for three-dimensional spatial quantities. The Einstein summation convention is used throughout, except where explicitly noted. The covariant derivative compatible with $g_{\mu\nu}$ is written as $\nabla_{\mu}$, and the covariant derivative compatible with the spatial metric $\gamma_{ij}$ is $D_{i}$. The flat metric is written as $\eta_{\mu\nu}$ and the flat scalar Laplacian is written as $\nabla^{2}$. Conformally scaled quantities are designated with either a tilde or bar, depending on the rescaling and will be noted in the text. All units are geometrized, $c = G = 1$. The Riemann tensor is defined as:

$$R^{\alpha}_{\beta\mu\nu} = \partial_{\mu} \Gamma^{\alpha}_{\beta\nu} - \partial_{\nu} \Gamma^{\alpha}_{\beta\mu} + \Gamma^{\alpha}_{\lambda\mu} \Gamma^{\lambda}_{\beta\nu} - \Gamma^{\alpha}_{\lambda\nu} \Gamma^{\lambda}_{\beta\mu},$$  \hspace{1cm} (A.1)

where $\Gamma^{\alpha}_{\mu\nu}$ are the Christoffel symbols corresponding to $g_{\mu\nu}$. The extrinsic curvature is defined as in York [176]:

$$K_{\mu\nu} = -\frac{1}{2} L_{\vec{n}} \gamma_{\mu\nu},$$  \hspace{1cm} (A.2)

where $L_{\vec{n}}$ is the Lie derivative along the normal, $n_{a}$. The spatial Riemann tensors are written as $(3)R$. The convention for the fourth Weyl Scalar, $\Psi_{4}$, is chosen to be

$$\Psi_{4} = +C_{\alpha\beta\gamma\delta} n^{\alpha} \bar{m}^{\beta} n^{\gamma} \bar{m}^{\delta},$$  \hspace{1cm} (A.3)

where $C_{\alpha\beta\gamma\delta}$ is the antisymmetric part of the Riemann tensor, and $n^{\alpha}$ and $\bar{m}^{\beta}$ are two basis vectors of the null tetrad, see Section 3.2.

**Simulations:** All calculations of final mass ($M_{h}$) and spin ($a/M_{h}$) reported in this dissertation are performed using the horizon method of Section 3.1. These values are also
checked against the calculation of mass and spin from $\Psi_4$, see Section 3.2. All calculations of the final kick of a BH are done using $\Psi_4$ and conservation of momentum. The ADM mass of the system, $M_{\text{adm}}$, is calculated through the initial data, see Equation 2.50. The total initial Christodoulou mass of the system is normalized to be $M = m_+ + m_- = 1.0$, accounting for both the irreducible mass of the BHs and their spins. The total initial angular momentum is given by the sum of the total orbital and spin angular momentum,

$$\vec{J} = \vec{L} + \vec{S}_+ + \vec{S}_-,$$

and is normalized with the ADM mass of the system, $\vec{J}/M_{\text{adm}}^2$. All simulations are initially oriented such that the initial orbital angular momentum, $\vec{L} = \vec{d} \times \vec{p}$, is in the $+\hat{z}$-direction.

All simulations presented in this dissertation can be described uniquely by six different initial properties: separation ($d/M$), mass ratio ($m_1/m_2$), impact angle ($\theta$), orbital angular momentum ($\vec{L}$), spin magnitudes ($S_\pm$), and spin orientation. The impact angle is the angle between the initial momentum vector and the vector connecting the two BHs initially. The orbital angular momentum is given by

$$|\vec{L}| = |\vec{d} \times \vec{P}| = |d||P| \sin \theta = |d||P_y|$$

(A.5)

Therefore, specifying the initial momentum is tantamount to specifying the initial orbital angular momentum.

In Chapter 4, the separation, mass ratio, and impact angle are kept fixed for all runs: $d/M = 10$, $m_1/m_2 = 1.0$, and $\theta = 26.565^\circ$. The spin orientation is always within the orbital plane, perpendicular to the orbital angular momentum. The remaining parameters are the free parameters of this study: the spin ($S_+ = S_- = S$), the angle the spins make with the $\pm x$-axis ($\phi_\pm$), and the initial orbital angular momentum ($\vec{L}$).

In Chapter 5, the separation and mass ratio are held constant for all runs: $d/M = 10$ and $m_1/m_2 = 1.0$. All spins are aligned or anti-aligned with the initial orbital angular momentum, allowing us to find the total angular momentum, $J = L + S_+ + S_-$. A given spin configuration, $S/M^2 = (m_1 + m_2)/(2m)^2 = (a_1/m + a_2/m)/4$, and impact angle, $\theta$, is chosen from the range $S/M^2 = -0.4$ to 0.4 and $\theta = 6^\circ$ to 90$^\circ$, respectively. For each combination of $S/M^2$ and $\theta$, the initial angular momentum $\vec{L}$ is varied.

In Chapter 6, the only free parameter is the initial angular momentum, $J/\mu M$. All other parameters are kept fixed: $d/M = 30$, $m_1/m_2 = 3$, $\theta = 90^\circ$, and $a_\pm/m_\pm = -0.3$ anti-aligned with $\vec{L}$. 

Appendix B

Post-Newtonian Evolution

The most astrophysically relevant configuration for a binary system is one in which the binaries are in a quasi-circular orbit with very low eccentricity. Even if a system has some non-zero eccentricity initially, it is believed that due to the radiation reaction force, this eccentricity will be shed quickly (in the form of gravitational waves) and circularize. Therefore, when generating gravitational waves via numerical simulations, quasi-circular parameters for the momentum, $P_i$, in Equation 2.43, need to be specified to initiate the binary for a given separation and spin configuration. There are several methods to do this, including an effective potential method [24, 64], and quasi-equilibrium methods [86]. A recent, iterative method has been proposed by Pfeiffer et al. [138] which by evolving a few orbits with a full numerical simulation, calculating the eccentricity, and then trying again until the desired eccentricity is reached, results in very low eccentricity quasi-circular orbits. However, this method is very expensive computationally since a few orbits can take several hours or even days, depending on the initial separation and resolution. These are not the methods used by the PSU-GATech NR group, however, who utilize post-Newtonian (PN) approximations to generate the initial parameters. We do this in two ways. The first uses the 3PN equation for the angular momentum of a binary system with spin [69, 110]:

$$\frac{J_{z,arb}}{\mu M} = \frac{1}{2\sqrt{\gamma}} + 2\sqrt{\gamma} + \left( \frac{5}{2} - \frac{9\eta}{2} \right) \gamma^{3/2} + \left( \eta^2 + \frac{205\pi^2}{128} - \frac{26063}{840} \eta + 4 \right) \gamma^{5/2}, \quad (B.1)$$

$$\frac{J_{z,spin}}{\mu M} = -\frac{1}{4} \gamma \sum_{i=1}^2 \chi_i \hat{s}_{i,z} \left( 12 \frac{m_i^2}{M^2} + 8\eta \right) - \frac{3}{4} \eta \chi_1 \chi_2 \gamma^{3/2} (\hat{s}_1 \cdot \hat{s}_2 - 3\hat{s}_{1,z}\hat{s}_{2,z}), \quad (B.2)$$

$$J_{z,tot} = J_{z,orb} + J_{z,spin} = rp_t, \quad (B.3)$$
where $S_i = \chi_i m_i^2 \hat{s}_i$, $\gamma = M/r$, $M = m_1 + m_2$ is the total mass of the system, $\mu = m_1 m_2 / M$ is the reduced mass, and $\eta = \mu / M = m_1 m_2 / M^2$ is the symmetric mass ratio.

The tangential momentum component, $p_t$, is then used to specify the momentum in the Bowen-York extrinsic curvature (Equation 2.43). This method has the advantage that for most spin configurations, low eccentricity initial parameters can be found. The main drawback however, is that the eccentricity is still non-negligible. It also only gives a term for the tangential momentum, and true quasi-circular orbits have a radial component of the momentum. These two drawbacks are remedied by a full evolution of the Taylor Expanded 3PN equations of motion with a 3.5PN radiation reaction force. By evolving the position, momenta, and spins of the binary system, a very low eccentricity can be achieved. However, the lower eccentricity for many initial configurations comes at a price, and the trade-off is that the method is not useful for many spin configurations and high mass ratios. The PN evolution method also has the advantage that it can be used to understand the zoom-whirl dynamics as discussed in Chapter 6, with many of the figures from that chapter being generated with the PN evolution code.

The 3PN Hamiltonian and radiation reaction force are found in concise form from Buonanno et al. [46] and will be presented below. This method was initially implemented by Husa et al. [103] who found that the eccentricity was decreased by a factor of 5 for a $d/M = 11$, non-spinning, and equal-mass BBH system as compared to simulation with initial parameters as in Equation B.1. Further, Walther et al. uses a modified PN evolution code [171] and compares several methods ($J_z$ Equation B.1, 3PN Taylor Expanded PN evolution, and 3PN Effective One Body (EOB) PN evolution).

## B.1 3PN Hamiltonian

A binary system can be described by four vector quantities comprising a *state vector*, the difference in the position of the particles, $X = X_1 - X_2$, the coordinate momentum, $P = P_1 = -P_2$, and the spins of the individual particles, $S_1$ and $S_2$. If we know these quantities initially, we can use the 3PN Hamiltonian and Hamiltonian’s equations of motion to find them at a later time. We begin by looking at the orbital part of the 3PN Taylor Expanded Hamiltonian and breaking it up into its contribution from each PN term [70, 71, 72, 105]:

$$H_{orb}(X, P) = \mu \left[ \hat{H}_N(q, p) + \hat{H}_{1PN}(q, p) + \hat{H}_{2PN}(q, p) + \hat{H}_{3PN}(q, p) \right], \quad (B.4)$$
where \( p := P_1/\mu = -P_2/\mu \), \( q := X/M \), and \( \mu = m_1 m_2/M \) is the reduced mass with \( M = m_1 + m_2 \), the total mass. The Newtonian and post-Newtonian Hamiltonians are given by

\[
\hat{H}_N = \frac{p^2}{2} - \frac{1}{q}, \tag{B.5}
\]

\[
\hat{H}_{1PN} = \frac{1}{8} (3\eta - 1)(p^2)^2 - \frac{1}{2} [(3 + \eta)p^2 + \eta (n \cdot p)^2] \frac{1}{q} + \frac{1}{2q^2}, \tag{B.6}
\]

\[
\hat{H}_{2PN} = \frac{1}{16} (1 - 5\eta + 5\eta^2)(p^2)^3
+ \frac{1}{8} [(5 - 20\eta - 3\eta^2)(p^2)^2 - 2\eta^2 (n \cdot p)^2 p^2 - 3\eta^2 (n \cdot p)^4] \frac{1}{q}
+ \frac{1}{2} [(5 + 8\eta)p^2 + 3\eta (n \cdot p)^2] \frac{1}{q^2} - \frac{1}{4} (1 + 3\eta) \frac{1}{q^3}, \tag{B.7}
\]

\[
\hat{H}_{3PN} = \frac{1}{128} (-5 + 35\eta - 70\eta^2 + 35\eta^3)(p^2)^4
+ \frac{1}{16} [(-7 + 42\eta - 53\eta^2 - 5\eta^3)(p^2)^3 + (2 - 3\eta)\eta^2 (n \cdot p)^2 (p^2)^2
+ 3(1 - \eta)\eta^2 (n \cdot p)^4 p^2 - 5\eta^3 (n \cdot p)^6] \frac{1}{q}
+ \left[ \frac{1}{16} (-27 + 136\eta + 109\eta^2)(p^2)^2 + \frac{1}{16} (17 + 30\eta)\eta (n \cdot p)^2 p^2
+ \frac{1}{12} (5 + 43\eta)\eta (n \cdot p)^4 \right] \frac{1}{q^2}
+ \left( \frac{85}{16} - \frac{3}{64}\pi^2 - \frac{7}{4}\eta \right) \eta (n \cdot p)^2 \right] \frac{1}{q^3} + \left[ \frac{1}{8} + \left( \frac{109}{12} - \frac{21}{32}\pi^2 \right) \eta \right] \frac{1}{q^4}, \tag{B.8}
\]

where \( n = q/q \). The spin contributions to the Hamiltonian come in two terms, a contribution from spin-orbit coupling and from spin-spin coupling [22, 23, 66]:

\[
H_{SO} = \frac{2 S_{eff} \cdot L}{R^3}, \tag{B.9}
\]

\[
H_{SS} = \frac{\mu}{2MR^3} [3(S_0 \cdot N)^2 - (S_0 \cdot S_0)], \tag{B.10}
\]

where \( N = X/R \), with \( R = |X| \), \( L = X \times P \) and the effective Spin, \( S_{eff} \) and \( S_0 \) are given by:

\[
S_{eff} := \left( 1 + \frac{3m_2}{4m_1} \right) S_1 + \left( 1 + \frac{3m_1}{4m_2} \right) S_2, \tag{B.11}
\]

\[
S_0 := \left( 1 + \frac{m_2}{m_1} \right) S_1 + \left( 1 + \frac{m_1}{m_2} \right) S_2. \tag{B.12}
\]
The full Hamiltonian is then given by the sum of these terms:

\[ H(X, P, S_1, S_2) = H_{orb}(X, P) + H_{SO}(X, P, S_1, S_2) + H_{SS}(X, P, S_1, S_2). \]  \( \text{(B.13)} \)

### B.2 Evolution equations

The evolution equation for a dynamical variable in the Hamiltonian formulation can be found by taking the Poisson bracket of the variable with the Hamiltonian, for example:

\[ \frac{dX}{dt} = \{X, H\}. \]  \( \text{(B.14)} \)

In this way, the Hamiltonian equations of motions can be found and are

\[ \frac{dX}{dt} = \frac{\partial H}{\partial P}, \]  \( \text{(B.15)} \)

\[ \frac{dP}{dt} = -\frac{\partial H}{\partial X}, \]  \( \text{(B.16)} \)

\[ \frac{dS_1}{dt} = \Omega_1 \times S_1, \]  \( \text{(B.17)} \)

\[ \frac{dS_2}{dt} = \Omega_2 \times S_2, \]  \( \text{(B.18)} \)

where \( \Omega_i = \frac{\partial H}{\partial S_i} \) and is given by \([23, 66, 164]\):

\[ \Omega_1 = \left[ \left( 2 + \frac{3m_2}{2m_1} \right) L + 3N(S_2 \cdot N) - S_2 + \frac{3m_2}{m_1}N(S_1 \cdot N) \right] \frac{1}{R^3}. \]  \( \text{(B.19)} \)

with \( \Omega_2 \) given by an interchange \( 1 \leftrightarrow 2 \) in the equation above. Taking the derivative of square of the magnitudes of \( S_i \) we see that

\[ \frac{dS_i^2}{dt} = 2S_i \cdot \frac{dS_i}{dt} = 2S_i \cdot (\Omega_i \times S_i) = 0, \]  \( \text{(B.20)} \)

since the quantity \( \Omega_i \times S_i \) is orthogonal to \( S_i \). In other words, the magnitude of the spin vectors are constant throughout the evolution.

### B.3 Radiation Reaction

The above evolution equations for a binary system are \textit{conservative}, meaning that the energy and angular momentum of the system is conserved. However, this can not be the true dynamics of the system, since any binary pair will release gravitational radiation
which carries away energy and momentum. To include this effect, we add a 3.5PN radiation reaction term to the momentum evolution equation (B.16):

\[
\frac{dP}{dt} = -\frac{\partial H}{\partial X} + F.
\] (B.21)

The radiation reaction force, \( F \), has the form [46]:

\[
F = \frac{1}{\omega |L|} \frac{dE}{dt} \mathbf{P} + \frac{8}{15} \eta^2 \nu_\omega^3 \left[ \left( 61 + 48 \frac{m_2}{m_1} \right) \mathbf{P} \cdot \mathbf{S}_1 + \left( 61 + 48 \frac{m_1}{m_2} \right) \mathbf{P} \cdot \mathbf{S}_2 \right] \mathbf{L},
\] (B.22)

where \( \omega = \dot{\phi} = \frac{V}{R} \) and \( \nu_\omega := (GM\omega)^{1/3} \). The change in energy, \( dE/dt \) has the form [29, 30, 31]:

\[
\frac{dE}{dt} = -\frac{32}{5} \eta^2 \nu_\omega^{10} \left[ 1 + f_2(\eta) \nu_\omega^2 + (f_3(\eta) + f_{3SO}) \nu_\omega^3 + (f_4(\eta) + f_{4SS}) \nu_\omega^4 + f_5(\eta) \nu_\omega^5 + (f_6(\eta) + f_6 \ln(4v_\omega)) \nu_\omega^6 + f_7(\eta) \nu_\omega^7 \right].
\] (B.23)

The flux coefficients are given by

\[
f_2(\eta) = -\frac{1247}{336} - \frac{35}{12} \eta,
\] (B.24)

\[
f_3(\eta) = 4\pi,
\] (B.25)

\[
f_4(\eta) = -\frac{44711}{9072} + \frac{9271}{504} \eta + \frac{65}{18} \eta^2,
\] (B.26)

\[
f_5(\eta) = -\left( \frac{8191}{672} + \frac{583}{24} \eta \right) \pi,
\] (B.27)

\[
f_6(\eta) = \frac{6643739519}{69854400} + \frac{16}{3} \pi^2 - \frac{1712}{105} \gamma_e + \left( -\frac{134543}{7776} + \frac{41}{48} \pi^2 \right) \eta
\] - \frac{94403}{3024} \eta^2 - \frac{775}{324} \eta^3,
\] (B.28)

\[
f_7(\eta) = \left( -\frac{16285}{504} + \frac{214745}{1728} \eta + \frac{193385}{3024} \eta^2 \right) \pi,
\] (B.29)

\[
f_6 = -\frac{1712}{105},
\] (B.30)

\[
f_{3SO} = -\left( \frac{11}{4} + \frac{5 m_2}{4 m_1} \right) \frac{\lambda \cdot \mathbf{S}_1}{GM^2} - \left( \frac{11}{4} + \frac{5 m_1}{4 m_2} \right) \frac{\lambda \cdot \mathbf{S}_2}{GM^2},
\] (B.31)

\[
f_{4SS} = \frac{\eta}{48G^2m_1m_2} [289(\lambda \cdot \mathbf{S}_1)(\lambda \cdot \mathbf{S}_2) - 103\mathbf{S}_1 \cdot \mathbf{S}_2],
\] (B.32)

where \( \lambda = L/|L| \), and \( \gamma_e = 0.577215665 \) is Euler’s constant.

With the radiation reaction force included in the evolution equations, the method can now be implemented to obtain low eccentricity initial quasi-circular parameters.
The Matlab implementation that I coded uses a Runge-Kutta Fourth order accurate time integration scheme to evolve the 12 dynamical variables of the binary state vector, $\{X, P, S_1, S_2\}$. Generally, the radiation reaction force works slowly, so a large initial separation is needed to shed the eccentricity. A separation of 100M is too large, since the time it takes to reach a small separation is huge, and at the gain of a negligible difference in final parameters. For non-spinning and comparable mass ratios, a distance of 40M is appropriate. For initial parameters, the spin and separation are specified by the user, and the 3PN angular momentum equation (B.1) is used to calculate the initial momentum. Since the 3PN angular momentum method has low eccentricity to begin with, this is a decent choice for initial momentum. After the evolution is complete, determined by the desired separation initially specified, the final state of the system is rotated so that the binaries start on the $x$-axis, and the final momentum and spin are used as the momentum and spin parameters in the Bowen-York extrinsic curvature (Equation 2.43).

B.4 Results

In Figure B.1, there are different configuration binaries with the inspiral from an initial separation of 15M to 6M in the left panel, and the separation versus time in the right panel. The top row is for an equal-mass, non-spinning system. Initially there are 'wiggles' in the separation, which damp out as the binaries approach. This is exactly the behavior we expect and want. Figure B.1, middle row shows the same behavior with a mass ratio of $m_1/m_2 = 4$. When spin is added, the orbits are no longer confined to an orbital plane as long as $S_{\text{eff}}$ and $L$ are not parallel or anti-parallel ($dL/dt \propto S_{\text{eff}} \times L$). This is illustrated in Figure B.1, bottom row. There is also spin precession as in Figure B.2. Figure B.3 shows the separation versus time for two different full NR runs, one with initial data generated via Equation B.1 and the other with the PN evolution equations for an equal-mass, non-spinning, BBH system with initial separation 9M. Clearly, the PN evolution method is less eccentric. Figure B.4 shows the orbit and separation for an NR run with equal-mass, non-spinning system with initial separation $d/M = 16$, with the initial parameters being generated by the PN evolution code. This binary completes $\approx 20$ orbits before merger, and is the longest running simulation I have performed to date ($\approx 6,300M$). After about $400 - 500M$, the initial eccentricity is already shed, and the remaining trajectory is very circular.

There are several areas where the code is not sufficient for generating low eccentricity
Figure B.1. Post-Newtonian evolution of an equal-mass, non-spinning binary system from $r=15M$ to $r=6M$. Top Left panel shows the orbits of the two BHs starting from $r=12M$ to $r=6M$ to show detail. The right panel shows the separation vs. time for the system. Note the wiggles in the separation damp slowly as the BHs approach. The middle row is the same for a mass ratio of $m_1/m_2 = 4$. The bottom row is an equal-mass system with arbitrary spin. The BHs are no longer confined to the orbital plane due to the spin-orbit coupling.
Figure B.2. Spin precession for an equal-mass binary. $S_x, S_y, S_z$ (red, blue, pink) all precess. The light blue line is the magnitude of the spin and stays constant throughout the evolution.

Figure B.3. PN evolution (blue) and 3PN angular momentum (red) initial parameters used for a full NR run.
initial parameters. For one, from a technical standpoint, since the spins precess, the BHs are not confined to an orbital plane, and \( \mathbf{S}_1 \cdot \mathbf{S}_2 \) is not guaranteed to be constant throughout the simulation, if you want a specific spin configuration in the final state, it may not be possible with the PN evolution method. For spins aligned with the angular momentum and mass ratios greater than \( m_1/m_2 \sim 4 \), the 3PN Taylor Expanded Hamiltonian leads to initial parameters that are more eccentric than ones calculated from Equation B.1. Walther et al. finds similar conclusions, and states that use of the EOB Hamiltonian results in a decrease in the eccentricity for those types of systems [171]. Therefore, it may be worth the time to implement the EOB Hamiltonian equation of motions in the future.

In conclusion, knowing the initial state vector \((\mathbf{X}, \mathbf{P}, \mathbf{S}_1, \mathbf{S}_2)\), we can evolve these quantities with radiation reaction and the 3PN Hamiltonian equations of motion to find low eccentricity initial parameters. For comparable mass binaries and no spin, the eccentricity reduction can be as great as a factor of 5 compared to other methods. However, for other configurations, the Taylor expanded Hamiltonian is not sufficient in reducing the eccentricity, and use of the EOB Hamiltonian may help.
Appendix C

Matched Filtering

When a signal is detected at a gravitational wave detector, such as ground-based LIGO, or space-based LISA, the signal will consist of both a gravitational wave and noise. Since the amplitude of the expected gravitational waveform will be on the order of the noise of the detector, a template bank of waveforms generated via numerical relativity and post-Newtonian methods is crucial to the separate the signal from noise. Matched filtering is a method to check an incoming signal against the template bank. It gives a sense of how well the signal matches a template waveform taking the noise of the detector into account. The matching algorithm discussed in this chapter follows from Vaishnav et al. [168].

C.1 Matching

As discussed in Section 3.2 the gravitational wave content of the BBH system is contained in $\Psi_4$ and is related to gravitational strain by a second derivative in time as in Equation 3.21. The matched filtering analysis requires $h(f)$, the waveform in the frequency domain, and therefore we take the Fourier transform of Equation 3.21 directly after removing the spurious radiation from the waveform, leading to

$$h_+(f) = \frac{\mathcal{F}(\text{Re}(\Psi_4))}{-4\pi^2 f^2},$$

$$h_\times(f) = \frac{\mathcal{F}(\text{Im}(\Psi_4))}{4\pi^2 f^2},$$

where $\mathcal{F}(h(t)) = \int_{-\infty}^{\infty} h(t)e^{-2\pi ift}dt$ is the Fourier transform. No integrals of $\Psi_4$ need to be taken since $\mathcal{F}(d^n h(t)/dt^n) = (2\pi f)^n h(f)$ so no integration constants (as discussed in
Section 3.2.2) are introduced. Further, the integration constants add a linear function at + b to the strain whose Fourier transform is \( \mathcal{F}(at + b) = a(i/2\pi)\delta'(f) + b\delta(f) \), or in other words, the integration constants just add a contribution to the frequency domain at \( f = 0 \) which is removed in the calculation of \( h(f) \) to prevent divide by zero errors in Equations C.1 and C.2. Therefore, no issues with integration constants arise in the matched filtering analysis.

The scalar product of two time domain waveforms, \( h_1(t) \) and \( h_2(t) \), is given by

\[
\langle h_1|h_2 \rangle = 4\text{Re}\left\{ \int_{f_{\text{max}}}^{f_{\text{min}}} \frac{h_1(f)\tilde{h}_2(f)}{S_h(f)} df \right\},
\]

where \( S_h(f) \) is the noise curve associated with a given gravitational wave detector. The waveforms, \( h_1(t) \) and \( h_2(t) \), can be, for example, a template bank waveform, and an incoming signal at a wave detector. They could also be two different numerical relativity waveforms that will be compared. The value \( f_{\text{min}} \) is the initial frequency of the binary system, which depends on the spin and the initial separation and the value \( f_{\text{max}} \) is determined by the detector bandwidth.

The scalar product is the building block of the four matching techniques implemented. The first is called the maximum overlap or match statistic [136]. When the two waveforms are compared, they may have different starting times, meaning for instance that the time of merger is different for each. Therefore, one of the waveforms is time shifted until a maximum in the overlap is found. The overlap is the normalized scalar product of the two waveforms and is:

\[
O[h_1, h_2] = \frac{\langle h_1|h_2 \rangle}{\sqrt{\langle h_1|h_1 \rangle \langle h_2|h_2 \rangle}}.
\]

The time shift \( h_1(t) \rightarrow h_1(t + t_0) \) results in an additional term in the frequency domain of \( h_1(f) \) and the numerator of Equation C.4 becomes

\[
\langle h_1|h_2 \rangle = 4\text{Re}\left\{ \int_{f_{\text{min}}}^{f_{\text{max}}} \frac{h_1(f)\tilde{h}_2(f)e^{2\pi i t_0}}{S_h(f)} df \right\}.
\]

Then the overlap is evaluated for a range of \( t_0 \) and the maximum overlap is defined as

\[
O_{\text{max}}[h_1, h_2] = \max_{t_0} O[h_1, h_2].
\]

In addition to \( t_0 \), the arrival time of the signal, there is another extrinsic parameter of our incident waveform, its initial phase, \( \Phi \). It is therefore desirable to have an optimization over the two initial phases of the waveforms, \( \Phi_1 \) and \( \Phi_2 \). We begin by normalizing
our waveforms $e_{i,x} = h_{i,x}(f)/\|h_{i,x}(f)\|$ where $i = 1, 2$ and the norm is defined by the scalar product, Equation C.3. An orthonormal basis $[131, 151]$ is then defined to allow for angles other than $(\theta = 0, \phi = 0)$, one of which is $e_{i+}$, the other given as $e_{i\perp} = e_{i+} \times (f) / \|e_{i\perp}\|$. (C.7)

With the new basis, we can define a typical match [131], in which the phase of one waveform is kept constant, while maximizing over the other:

$$M_{\text{typ}} = \max_{t_0} \max_{\Phi_2} O[h_{1+}, h_2]$$

$$= \max_{t_0} \|O[e_{1+}, e_{2+}]^2 + O[e_{1+}, e_{2\perp}]^2\|. \quad \text{(C.8)}$$

We can also define matches in which we maximize over both phases, the best match [68], and maximize over one phase while minimizing over the other, the minimax match [68]. These are considered the best and worst match one could obtain when maximizing over a single phase, as is the case when a signal is detected and compared to a template bank waveform. The best match is defined as

$$M_{\text{best}} = \max_{t_0} \max_{\Phi_1} \max_{\Phi_2} O[h_{1+}, h_2]$$

$$= \max_{t_0} \left[ \frac{A + B}{2} + \left[ \left( \frac{A - B}{2} \right)^2 + C^2 \right]^{1/2} \right]. \quad \text{(C.9)}$$

and the minimax match as

$$M_{\text{minimax}} = \max_{t_0} \min_{\Phi_1} \max_{\Phi_2} O[h_{1+}, h_2]$$

$$= \max_{t_0} \left[ \frac{A + B}{2} - \left[ \left( \frac{A - B}{2} \right)^2 + C^2 \right]^{1/2} \right]. \quad \text{(C.10)}$$

In both cases, $A$, $B$, and $C$, are

$$A = \langle e_{1+} | e_{2+} \rangle^2 + \langle e_{1+} | e_{2\perp} \rangle^2, \quad \text{(C.11)}$$

$$B = \langle e_{1\perp} | e_{2+} \rangle^2 + \langle e_{1\perp} | e_{2\perp} \rangle^2, \quad \text{(C.12)}$$

$$C = \langle e_{1+} | e_{2+} \rangle \langle e_{1\perp} | e_{2+} \rangle + \langle e_{1+} | e_{2\perp} \rangle \langle e_{1\perp} | e_{2\perp} \rangle. \quad \text{(C.13)}$$
A matched filtering technique has been used by the PSU group in the past to compare waveforms with different resolutions, different initial angular momentum, and different inclination angles between observer and source [168]. More recently, Bode et al. used matched filtering to compare waveforms generated from the same simulation with initial data generated via different methods [34]. I have implemented the above algorithm in Matlab as part of the post-processing infrastructure of the PSU-GATech numerical relativity group.

### C.1.1 Detector Noise Curves

An important component of the matched filtering algorithm is the Power Spectral Density (PSD) of the associated wave detector, \( S_h(f) \). We use analytic PSDs for initial LIGO, enhanced LIGO, advanced LIGO [1] that are given by

\[
\text{initial LIGO : } S_h(f(x)) = 9 \times 10^{-46}[(4.49x)^{-56} + 0.16x^{-4.52} + 0.52 + 0.32x^2],
\]

\[
\text{enhanced LIGO : } S_h(f(x)) = 1.5 \times 10^{-46}[1.33 \times 10^{-27}e^{-5.5(lnx)2}x^{-52.6} + 0.16x^{-4.2} + 0.52 + 0.3x^2],
\]

\[
\text{advanced LIGO : } S_h(f(x)) = 10^{-49}\left[ x^{-4.14} - 5x^{-2} + 111\left( \frac{1 - x^2 + x^4/2}{1 + x^2/2} \right) \right], \quad (C.14)
\]

where \( x = f/f_0 \), and \( f_0 \) is 150 Hz, 178 Hz, and 215 Hz for initial, enhanced, and advanced LIGO respectively. We also have an analytic noise curve for LISA [11] given piecewise for \( u < 0.25 \)

\[
S_h(f) = \frac{8.08 \times 10^{-48}}{(2\pi f)^4} + 5.52 \times 10^{-41}, \quad (C.15)
\]

and for \( u \geq 0.25 \),

\[
S_h(f) = \frac{1}{R} \left( \frac{8.08 \times 10^{-48}}{(2\pi f)^4} + 5.52 \times 10^{-41} \right), \quad (C.16)
\]

where \( u = 2\pi f \tau \), \( \tau = 5 \times 10^6 \text{km}/c \) is the time it takes for light to travel down LISA’s arms, and

\[
R = \frac{1}{u^2} \left[ (1 + \cos^2(u)) \left( \frac{1}{3} - \frac{2}{u^2} \right) + \sin^2(u) + \frac{4\sin(u)\cos(u)}{u^3} \right]. \quad (C.17)
\]

See Figure C.1 for a plot of the noise curves versus frequency. We also have data for the PSDs of initial LIGO and advanced LIGO that can be interpolated into the frequency range of the system.
C.1.2 Physical Units

After working in geometrized units, finding the physical units of quantities becomes a non-trivial exercise. In this section, I will quickly outline how to take the quantities from the numerical relativity simulations, which are in units of $M_{\text{code}}$ and convert them to physical units. Note that for the matched filtering discussed in this chapter, the magnitude of the waveform does not contribute due to the normalization. However,
when looking at the signal to noise ratio (SNR),

$$\text{SNR} = \sqrt{\langle h| h \rangle},$$  \hspace{1cm} (C.18)

the correct physical units are critical to an accurate result.

Results from the MayaKranc code are scalable by the overall mass of the system, typically chosen to be some multiple of the mass of the sun, $\alpha M_\odot$. $M_{\text{code}}$ is generally 1.0 but need not be. Accordingly, the scaling factor of the system is then

$$M_{\text{scale}} = \alpha M_\odot / M_{\text{code}}.$$  \hspace{1cm} (C.19)

The way physical units enter the system are via $M_\odot$. The mass of the sun in various units is:

\[
M_\odot = 1.9889 \times 10^{30} \text{ kg} \\
= 4.9267 \times 10^{-6} \text{ s} \\
= 1.4770 \times 10^{3} \text{ m} \\
= 4.7866 \times 10^{-20} \text{ Mpc}
\]

where factors of $G$ and $c$ were used to change units between kg, m, and s. The two important quantities to give physical units to are the time and $\Psi_4$ since both are needed for the matched filtering. The time scale is straightforward, it is just

$$t_{\text{physical}} = t_{\text{code}} \times M_{\text{scale}}$$  \hspace{1cm} (C.20)

where $M_{\text{scale}}$ is in units of seconds. $\Psi_4$ is the second time derivative of the gravitational strain, $h$, which is unitless. Therefore, $\Psi_4$ has units $s^{-2}$ and

$$\Psi_{4\text{physical}} = \Psi_{4\text{code}} \times M_{\text{scale}}^{-2}$$  \hspace{1cm} (C.21)

where again $M_{\text{scale}}$ has units of seconds.

There is another subtlety with $\Psi_4$ that is needed when calculating the SNR. As the distance from the source to detector, $D$, increases, the signals falls off as $1/D$. Generally, $\Psi_4$ is known at finite extraction radii that is not equal to $D$. $\Psi_4$ needs to be rescaled once again to the distance in question. Taking $\Psi_{4\text{physical}}$ from Equation C.21 and multiplying by the extraction radii, $r$, in units of Mpc, gives a rough estimate of $\Psi_4$ at infinity. This
is then divided again by $D$ to find $\Psi_4$ at $D$. Succinctly, $\Psi_4$ at $D$ is

\[
\Psi_{4, atD} = \frac{r M_{scale}[\text{Mpc}]}{D[\text{Mpc}]} \times \Psi_{4, physical}.
\]  

(C.22)

With this, the matched filtering analysis and signal to noise ratio can be accomplished at different masses of the system and at different reference distances to get a complete analysis of the waveforms in question.
References


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Vita

James Healy

James Christopher Healy, son of James Joseph Healy and Christine Healy, was born in Livingston, NJ on January 11, 1984. He attended the University of Delaware in Newark, DE from 2002-2006 and graduated summa cum laude with a Bachelor of Science degree in Physics with a minor in Mathematics and Japanese. He started his graduate career at Penn State University in University Park, PA seeking a PhD in Physics. He began work with the numerical relativity group under Pablo Laguna and Deirdre Shoemaker in November 2007, and quickly learned the code infrastructure and started numerous research projects. He married his girlfriend of 10 years, Allison Fields, on September 27, 2009. James Healy is a member of Phi Beta Kappa Honor Society and received the Duncan Fellowship in Spring 2009.


