

# On the Initial Boundary Value Problem in Numerical Relativity

by

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### **Author's Declaration**

This thesis consists of material all of which I authored or co-authored: see Statement of Contributions included in the thesis. This is a true copy of the thesis, including any required final revisions, as accepted by my examiners.

I understand that my thesis may be made electronically available to the public.

## **Statement of Contributions**

Conner Dailey is the sole author of Chapters 1, 4, and 5.

Chapters 2 and 3 consist of previously published work that was submitted under the authorship of Conner Dailey, Niayesh Afshordi, and Erik Schnetter, but the vast majority of the material was written, edited, and authored by Conner Dailey.

## Abstract

The principal goal of this thesis is to properly understand, characterize, and numerically implement initial boundary value problems in numerical relativity. Throughout the history of solving Einstein's field equations on computers, boundaries have been mostly dealt with in an approximate way. For example, boundaries might be placed far away from strongly gravitating sources, where approximations like linearized gravity are valid. It has become necessary however to place boundaries in the strong gravity regime of a dynamical spacetime to model complicated and interesting physics, which necessitates a complete understanding of the initial boundary value problem of Einstein's field equations.

One motivation for this comes from a need to simulate black hole echoes. In classical general relativity, black holes are perfectly absorbing objects, where the mass of radially incoming wavepackets of matter or gravitational waves is absorbed by the black hole. Thus conclusive evidence of modifications to general relativity, such as quantum gravity, could include partial reflections of radially incoming wavepackets, called black hole echoes. To properly understand the modifications this would bring to detectable gravitational wave signals, we require simulations where reflecting boundary conditions are imposed close to the horizon of a black hole. Another motivation comes from recent advances in Cauchy characteristic matching, which combines state of the art numerical techniques to obtain physically accurate gravitational waveforms from simulations. This can allow numerical relativists to dramatically save on the computational cost of black hole merger simulations, but only if boundaries can be placed in the strong gravity regime.

This thesis presents advances in simulating initial boundary value problems in numerical relativity. Starting with spherical symmetry, a framework for reflecting a scalar field in a fully dynamical spacetime is developed and implemented numerically using the Einstein-Christoffel formulation. The evolution of a wave packet and its numerical convergence, including when the location of a reflecting boundary is very close to the horizon of a black hole, is studied. Next, this approach is generalized to spacetimes with no symmetries and implemented numerically using the generalized harmonic formulation. The evolution equations are cast into a summation by parts scheme, which seats the numerical method closer to a class of provably numerically stable systems. State of the art numerical methods are demonstrated, including an embedded boundary numerical method that allows for arbitrarily shaped domains on a rectangular grid and even boundaries that evolve and move across the grid. As a demonstration of these frameworks, the evolution of gravitational wave scattering off of a boundary either inside or just outside the horizon of a black hole, is studied. Finally, a boundary condition framework designed to control quasi-local energy flux is proposed motivated by examples from electromagnetism.

## Acknowledgements

First and foremost I must thank my main supervisor Niayesh Afshordi. Had he not advocated for me before he had even met me in person, I would likely not have started my Ph.D. at the University of Waterloo. Throughout my Ph.D. studies, he has done an excellent job at guiding me in the right direction and curating my interests.

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I am very thankful for many interesting and helpful interactions with experts in the field of strong gravity and numerical methods, including Luis Lehner, Richard Epp, and all of those serving on my examining committee. I am grateful to the members of the Strong Gravity group at the Perimeter Institute for many interesting talks and for listening and considering my own work on the occasions that I presented to the group.

This work was made possible with the Julia programming language [1], where the spherically symmetric work was accomplished using the numerical integration package `DifferentialEquations.jl` [2] and the three dimensional work was developed using the grid parallelization package `ParallelStencil.jl` [3] and the tensor type package `Tensorial.jl` [4].

My time as a Ph.D. student was made incredibly memorable by a long list of great friends from the Waterloo Center for Astrophysics and the Perimeter Institute. I am continually fostered and supported by my loving family, thanks to my mother Marci Burke, my father Morgan Dailey, and my sister Lily Dailey for always believing in me and pushing me to be my best.

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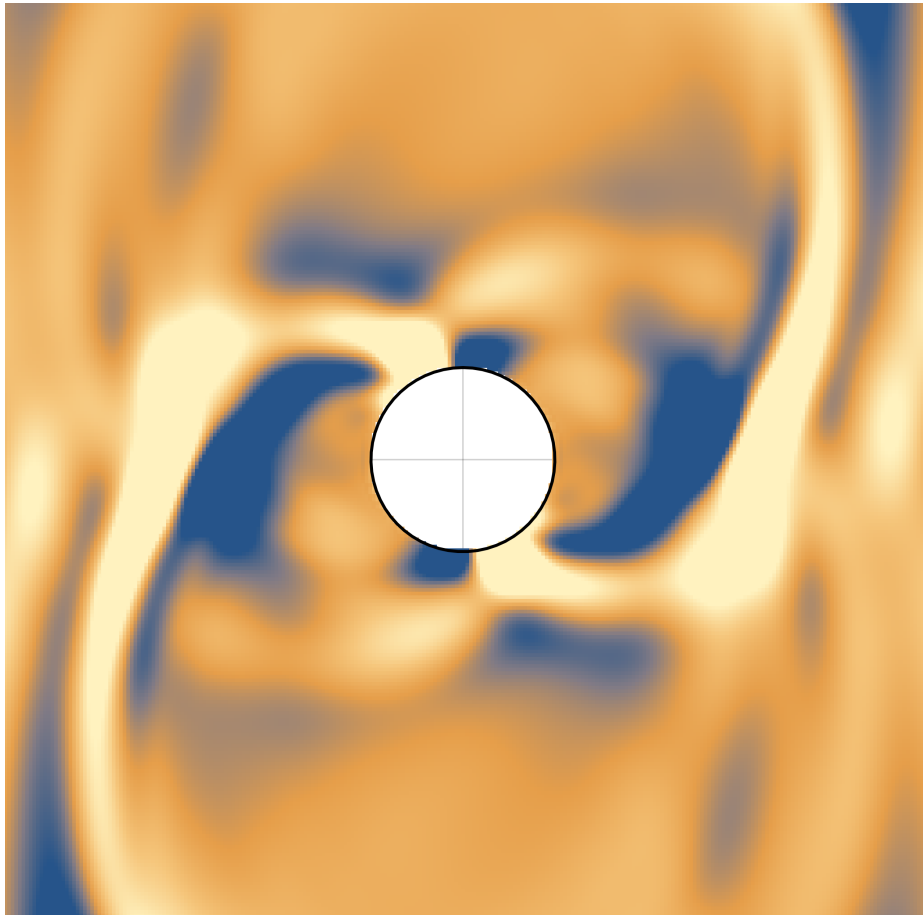
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# Chapter 1

## Introduction

### Preface

This chapter serves to introduce the reader to the various subjects and mathematical tools that tend to be taken for granted in the numerical relativity community, but may not be familiar to the layman or even the average physicist. As two of the following chapters in this thesis include work that was directly published to an audience within the numerical relativity community, this chapter serves to make this thesis more accessible to a broader audience, and to make it as self-contained as possible. References to ‘we’ in this chapter refer to the author of this thesis and the reader.

Section [1.1](#) discusses the motivations behind demonstrating successful and numerically stable initial boundary value problems in numerical relativity. Section [1.2](#) introduces the reader to the mathematical tools widely used in subsequent chapters. Section [1.3](#) introduces the concept of hyperbolicity and discusses the importance of casting evolution equations in a symmetric hyperbolic form. Section [1.4](#) introduces the modern numerical methods used to solve systems of partial differential equations in a numerically stable fashion. Finally, Section [1.5](#) discusses two symmetric hyperbolic formulations of numerical relativity, both of which are demonstrated as a numerically stable evolution in subsequent chapters.

## 1.1 Motivations

The motivation to pursue a proper way to formulate and numerically implement initial boundary value problems in numerical relativity comes from a need to model new and interesting physical phenomena on surfaces located in the strong gravity regime of a dynamical spacetime. One example of this comes from black hole echoes, which could potentially be the first observational signatures of quantum phenomena or other phenomena beyond general relativity near the horizons of black holes. Another example comes from new numerical methods that can allow for reduced computational cost of large scale simulations of merging black holes. Finally, the simulation of generic compact objects larger than black holes is discussed as a possible use case for initial boundary value problems with the boundary surface modeling the surface of any compact object.

### 1.1.1 Black Hole Echoes

In classical general relativity, black holes have horizons that are one-way surfaces. That is to say that the horizon is a surface that traps light rays within a closed region. Once the horizon has been crossed from the outside, the only trajectories that can reach the outside again are spacelike, requiring a superluminal speed. In this sense, the horizon is a perfectly absorbing surface for particles and waves. It is natural to think that modifications to general relativity could dictate different physics at the horizon, such as making the horizon surface not perfectly absorbing, and thus there would be some effective reflection of incident waves. The observable signals resulting from this potential reflection near the horizon of a black hole are called black hole echoes.

Modifications to general relativity are important to consider, as understanding the observable differences can lead to the discovery of new physics. It is well known in the physics community that gravity must be modified at small scales to properly be unified with quantum field theory. Such theories of quantum gravity are one such modification to general relativity that could lead to the production of black hole echoes. Attempts to solve problems in general relativity, such as the cosmological constant problem [5] or the black hole information paradox [6], also suggest Planck scale modifications near the horizons of black holes, potentially producing black hole echoes.

There is a large set of work dedicated to the study and modeling of black hole echoes. Early studies took a phenomenological approach to generating a template of what the echoing gravitational wave merger signals might look like at a detector [7, 8]. Some studies considered linearized gravity and developed reflecting boundary conditions that can be

applied on an approximate stage. Some studies restricted to non-spinning black holes [9, 10, 11], while some others generalized this analysis to spacetimes similar to a spinning black hole [12, 13, 14, 15]. Boundary conditions and analysis based on more realistic quantum gravity motivated assumptions are considered in [16]. The one thing all of these studies have in common however is the use of some sort of approximation, be that perturbation theory or linearized gravity.

One concrete example of black hole echoes considered in the literature are the so-called Boltzmann echoes [16, 17, 18]. Starting from the assumption that black holes are quantum objects that follow standard rules of quantum mechanics and thermodynamics in the small region near their horizons, it is derived in three independent ways in [18] that the coefficient of reflectivity of incident gravitational waves depends on the Hawking temperature and the wave frequency. In particular, it is shown that quantum black holes cannot be perfectly absorbing because that would imply a violation of unitarity, which would clash with standard results in quantum mechanics. In this way, black hole echoes seem to be a natural result of the extension of classical gravity to quantum gravity.

Considering modifications to general relativity is not the only way to generate echoes however. Instead, objects that are not dense enough to collapse to a black hole, but still compact enough to be near the scale of a black hole, can generate echoes as well. There are a large class of compact objects that have been proposed, including fuzzballs [6, 19], gravastars [20], and aether black holes [5]. All compact objects will have a specific surface structure and underlying physics that can potentially have observable differences in comparison to standard black holes. In the context of black hole echoes, those compact objects that have an effective reflecting surface are those that would produce a gravitational wave signal close to that of the proposed black hole echo models.

Black hole echoes are well motivated, and their discovery would be a smoking-gun for some sort of modified understanding to the objects responsible for gravitational wave events. As discussed, much work has been done to model black hole echoes, but these analyses are missing a complete nonlinear description. Phenomenological or linearized approximations are not adequate to understand and simulate physically accurate echoes of gravitational waves. This is because the echo generating surface is necessarily in the strongly gravitating region of the spacetime, where approximate methods tend to break down. This is why a complete nonlinear understanding of what it means to reflect gravitational radiation and a proper implementation to simulate black hole echoes using the complete nonlinear system of Einstein's field equations is needed. This thesis is dedicated to defining what this means and making it numerically feasible to implement.

### 1.1.2 Cauchy Characteristic Matching

Another problem with classical general relativity is that Einstein’s field equations are an incredibly difficult system to solve numerically. It is not uncommon for an accurate solution to require an immense amount of time and computing resources. To improve on this daunting computational cost, many clever numerical methods and frameworks have been devised and demonstrated over the years.

The earliest studies in numerical relativity were restricted to spherical symmetry as computer technology did not yet allow for systems of higher dimension. As technology improved, axial symmetry became feasible, but posed many numerical challenges. Presently, three dimensional simulations of black hole mergers have been demonstrated many times, and gravitational waveforms from many different types of merging objects have been cataloged, allowing for gravitational wave detectors to search and constrain their measurements.

In order to obtain the observable gravitational wave signal from a simulation, two different types of evolution formalisms are typically adopted, Cauchy evolution and characteristic evolution. Cauchy evolution is achieved by slicing the spacetime into spacelike hypersurfaces and an evolution system comprising Einstein’s field equations in a particular formulation are evolved numerically from one spatial slice to the next. In contrast, characteristic evolution works by slicing the spacetime on a series of null hypersurfaces that reach all the way to null infinity. The coordinates installed on these slices are compactified so that future null infinity can be properly evolved and modeled as a perfectly absorbing boundary even on a finite grid. The characteristic evolution can only be achieved where null caustics are not present, as due to the null foliation, such crossing of the null hypersurfaces would create coordinate singularities, and thus characteristic evolution cannot be used to evolve the strong gravity region. A complete procedure to extract gravitational wave information at null infinity includes simulating the strong gravity region with a Cauchy evolution scheme, using it to generate outgoing metric information on a timelike worldtube boundary, then using a characteristic evolution to advance this information out to null infinity. This is known in the literature as Cauchy characteristic evolution, and is visualized in Figure 1.1.

Unfortunately, even this complicated evolution scheme is not good enough to give physically realistic gravitational waveforms. This is because Einstein’s equations are nonlinear, and thus nonlinear effects such as wave scatter off of spacetime curvature, and even wave self-scatter, are present. This means that outgoing gravitational waves are not purely outgoing always, as some of the wave’s energy may scatter back into the strong gravity regime that contains the dynamical sources. Thus these sources are continually receiving feedback from their own outgoing wavefronts. Cauchy characteristic evolution does not properly

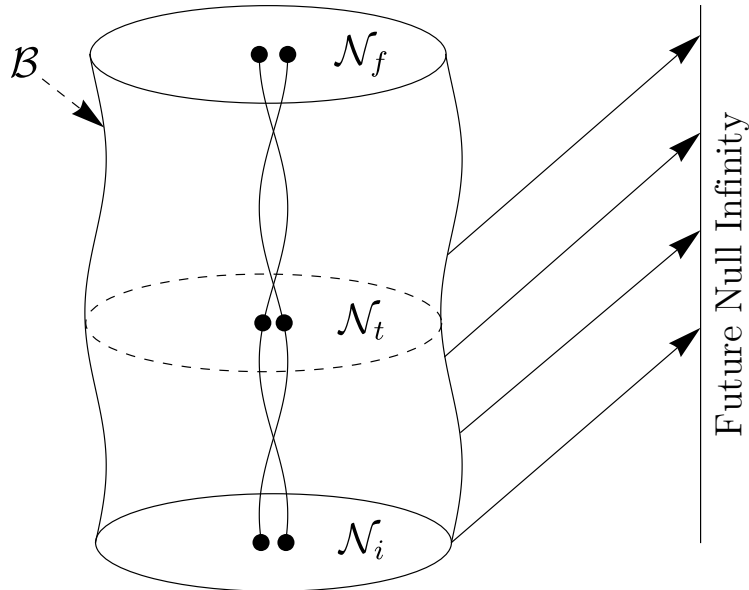


Figure 1.1: Diagram of a typical binary black hole simulation performed via Cauchy characteristic evolution, where time runs on the vertical, the 3-space is horizontal, and null rays run along  $45^\circ$  lines. The simulation begins on the initial spatial Cauchy slice  $\mathcal{N}_i$  and advances to the final slice  $\mathcal{N}_f$ . Black points represent the two orbiting black holes within these Cauchy slices acting as the sources of outgoing gravitational waves. Outgoing metric information is collected at the outer boundary worldtube  $\mathcal{B}$  and injected into a characteristic evolution scheme based on a null foliation of spacetime, which then advances the outgoing metric information to future null infinity where gravitational waveforms can be extracted.

model this, as it is a one way evolution, taking the timelike worldtube data out to infinity without any ingoing scatter affecting the sources. This is rectified by a newly demonstrated numerical mechanism deemed Cauchy characteristic matching [21]. This method evolves the characteristic evolution alongside the Cauchy evolution, and allows for gravitational wave scatter in the characteristic evolution zone to carry back toward the sources, and that scattering information is fed back into the Cauchy evolution as incoming boundary conditions. In this way, accurate gravitational waveforms can be extracted at infinity that are more physically realistic and just as accurate as if the Cauchy evolution domain was simply made much larger. The computational efficiency of Cauchy characteristic matching based evolution schemes is dictated largely by the Cauchy evolution, and so shrinking the size of the Cauchy evolution domain allows for simulations with significantly reduced computational cost.

This is another motivation for the endeavor for a complete understanding of the initial boundary value problem in numerical relativity. Shrinking the Cauchy evolution domain brings the boundary worldtube closer to the strong gravity regime, where nonlinear effects increase the likelihood of numerical instability. This thesis demonstrates the ability to evolve spacetimes in a numerically stable fashion even when boundaries are placed in the strong gravity regime, close to the horizon of a black hole for example. In principle, the numerical methods derived and demonstrated here can allow for the further shrinking of Cauchy evolution domains, that when evolved in the fashion of Cauchy characteristic matching, can give physically realistic and accurate gravitational waveforms with dramatically increased computational efficiency.

### 1.1.3 Compact Objects

Another subject of significant interest in the relativity community is the study of compact objects. These represent a class of astronomical objects different from black holes that could be responsible for measurements taken by experiments that probe general relativity.

An example would be the events that are measured by gravitational wave detectors like LIGO, that are thought to originate from the merger of black holes and neutron stars, but large uncertainties in these measurements may allow for a consistent origin from the merger of other types of compact objects. Another example is the measurements taken by the Event Horizon Telescope, which produces radio wave images of objects also thought to be black holes, but large uncertainties in these images could allow for a consistent object that does not have a horizon like a black hole does, and could be a compact object with an extent slightly larger than the Schwarzschild radius for example.

As mentioned earlier, there are a large class of compact objects that have been proposed, including fuzzballs [6, 19], gravastars [20], and aether black holes [5]. The initial boundary value problem in numerical relativity provides a way to simulate the surfaces of these compact objects with or without assumptions about their interior region. As long as the physics on the surface are given, such as how the boundary surface evolves with time and the boundary conditions on that surface, then any type of compact object can be simulated in principle. This would allow studies of the mergers of compact objects to be done in a much simplified manner, allowing numerical relativists to increase our understanding in the observable differences that these objects would make in detectors that probe general relativity, which may not necessarily fit the black hole echo model.

## 1.2 Prerequisites and Notation

As this thesis pertains to general relativity, some concepts in differential geometry are required. This section introduces some necessary mathematics and notation that will be used throughout the main material. Much of this comes directly from [22], and this is a good general reference for mathematical tools in relativity that may not be familiar to the reader. Topics more specific to numerical relativity and the  $3 + 1$  formalism come from [23] and [24], which are good starting points for those who want more detail in these areas. As is very common in the numerical relativity community, we use a unit system where  $G = c = 1$  so that most unitful quantities can be expressed relative only to a mass scale and all light-like trajectories propagate at speed 1.

### 1.2.1 Index Notation

To make the large sums and the complicated dimensionality of mathematical objects easier to deal with, Einstein summation convention and notation is used to a large degree. In this framework, mathematical objects are expressed in terms of symbols and their indices

$$T, T^\mu, T_\mu, T_{\mu\nu}, T^{\mu\nu}, T^\alpha_{\mu\nu}, \dots \quad (1.1)$$

An index is called a covariant (or lower) index if it is written as a subscript, and a contravariant (or upper) index if it is written as a superscript. The index represents the set of coordinate components needed to describe the object on a given dimension of manifold. In this work, indices written with Greek letters stand for the set of four coordinates chosen to describe a four dimensional spacetime manifold. This set of coordinates can hold the usual Cartesian component names  $x^\mu = (t, x, y, z)$  or any other set of names for different types of coordinate systems, such as spherical coordinates for example. The object  $T$  has only one component, while the object  $T^\mu = (T^t, T^x, T^y, T^z)$  requires four components. The number of components of an object is its rank (the number of indices needed to denote the object) times the dimension of the manifold.

Any set of two indices of any object can be separated into a symmetric and an anti-symmetric part

$$T_{\mu\nu} = T_{(\mu\nu)} + T_{[\mu\nu]}, \quad (1.2)$$

where parentheses and square brackets denote the symmetrization and anti-symmetrization operations respectively

$$T_{(\mu\nu)} = \frac{1}{2}(T_{\mu\nu} + T_{\nu\mu}), \quad T_{[\mu\nu]} = \frac{1}{2}(T_{\mu\nu} - T_{\nu\mu}). \quad (1.3)$$

These operators can be generalized to an arbitrary number of indices, but is beyond the scope of this thesis. One important object,  $g_{\mu\nu}$ , is called the metric tensor. It measures an arbitrary infinitesimal distance  $ds$  in terms of the chosen coordinates:

$$ds^2 = g_{\mu\nu} dx^\mu dx^\nu . \quad (1.4)$$

In this expression, Einstein summation convention is used, where a multiplication of two objects with a repeated upper and lower index label denotes a sum over all of the components spanned by that index (i.e.  $A^\mu B_\mu = A^t B_t + A^x B_x + A^y B_y + A^z B_z$ ). In the context of flat empty space, the metric can take the form of the Minkowski metric, which describes how to measure distances in flat Minkowski space

$$g_{\mu\nu} = \eta_{\mu\nu} = \text{diag}(-1, 1, 1, 1) , \quad (1.5)$$

which defines the metric signature chosen for the rest of this thesis. This type of metric is called Lorentzian because of the one negative metric component for time, which forces the failure of the metric norm to be positive definite. That is to say that the magnitude of an arbitrary one index object is not necessarily positive. A one index object  $u^\mu$  is classified based on the sign of its norm:

$$g_{\mu\nu} u^\mu u^\nu \begin{cases} < 0 & \text{timelike} \\ = 0 & \text{null or lightlike} \\ > 0 & \text{spacelike} \end{cases} . \quad (1.6)$$

At a given spacetime point (or event)  $A$ , the set of all null one index objects at  $A$  form two geometrical cones, the future directed ones form the future light cone and the past directed ones form the past light cone. Points within these cones are causally connected to  $A$ , as they are connected by a trajectory requiring a speed  $v \leq 1$ .

The indices of an object can be made covariant by *lowering* them with the metric  $g_{\mu\nu}$ :

$$T_{\alpha\beta} = g_{\alpha\mu} T^\mu{}_\beta , \quad (1.7)$$

and they can be made contravariant by *raising* them with the matrix inverse of the metric:  $g^{\mu\nu} \equiv (g_{\mu\nu})^{-1}$ :

$$T^\alpha{}_\beta = g^{\alpha\mu} T_{\mu\beta} . \quad (1.8)$$

When an object expression is written with an equality, there are two types of index labels, those that are repeated and summed (called summed indices) and those that are not (called free indices). The number of free indices on each side of the equality must match or else the expression is not interpretable. We refer to the symbols in these expressions as ‘objects’ because we have yet to assume they have any particular transformation properties, which we will do next.

## 1.2.2 Tensors

On a manifold, we are always free to choose an arbitrary set of coordinates with which to express the functions that represent the coordinate components of objects. If we have an expression for an object in terms of one set of coordinates  $x^\mu = (t, x, y, z)$ , we are free to re-express it in terms of a different set of coordinates  $x'^\mu = (t', x', y', z')$ . In order to transform objects from one coordinate system to the next, we will need the Jacobian matrix and its determinant:

$$\Lambda^\mu{}_\nu = \frac{\partial x'^\mu}{\partial x^\nu}, \quad \Lambda = \det(\Lambda^\mu{}_\nu). \quad (1.9)$$

An index-less object that changes under a coordinate transformation as

$$T'(x'^\mu) = T(x^\mu), \quad (1.10)$$

is called a *scalar*. It is important to emphasize that this did not need to be the case. In fact, there are a class of *scalar densities* of weight  $w$  that instead transform as

$$T'(x'^\mu) = \Lambda^w T(x^\mu), \quad (1.11)$$

so although an object may be *scalar-valued* in the sense that it only requires one component to describe, it may not necessarily transform as a scalar. An object with one contravariant index is called a *vector* if

$$T'^\alpha(x'^\mu) = \Lambda^\alpha{}_\beta T^\beta(x^\mu), \quad (1.12)$$

while if an object that transforms as

$$T'_\alpha(x'^\mu) = (\Lambda^{-1})_\alpha{}^\beta T_\beta(x^\mu), \quad (1.13)$$

it is called a *covector* or a dual vector, where  $(\Lambda^{-1})_\alpha{}^\beta$  is the matrix inverse of the Jacobian. In general an object is called a type  $(n, m)$  *tensor* if it has  $n$  contravariant indices,  $m$  covariant indices, and it transforms as

$$T'^{\alpha_1 \dots \alpha_n}{}_{\beta_1 \dots \beta_m}(x'^\mu) = \Lambda^{\alpha_1}{}_{\mu_1} \dots \Lambda^{\alpha_n}{}_{\mu_n} (\Lambda^{-1})^{\nu_1}{}_{\beta_1} \dots (\Lambda^{-1})^{\nu_m}{}_{\beta_m} T^{\mu_1 \dots \mu_n}{}_{\nu_1 \dots \nu_m}(x^\mu). \quad (1.14)$$

This framework is powerful, as it allows for the concept of *tensor equations*. If both the left hand side and right hand side of the equality in a equation transform as a tensor, then that equation is valid in any coordinate system. As we consider physical laws to be independent of coordinate choices, it is important for our physical laws to be expressed in terms of tensor equations.

The partial derivative can be seen to transform as a covector by applying the chain rule:

$$\frac{\partial}{\partial x'^\nu} = (\Lambda^{-1})_\nu{}^\mu \frac{\partial}{\partial x^\mu} \equiv (\Lambda^{-1})_\nu{}^\mu \partial_\mu. \quad (1.15)$$

However, the partial derivative of a vector for example does not transform as a type  $(1, 1)$  tensor

$$\frac{\partial}{\partial x'^\beta} A'^\alpha = \Lambda^\alpha{}_\nu (\Lambda^{-1})_\beta{}^\mu \partial_\mu A^\nu + (\Lambda^{-1})_\beta{}^\nu A^\mu \partial_\mu \Lambda^\alpha{}_\nu. \quad (1.16)$$

We introduce the operator  $\nabla_\mu$ , called the *covariant derivative*, by demanding that when it is applied to a type  $(n, m)$  tensor, the result is always a type  $(n, m + 1)$  tensor. When applied to an arbitrary vector field  $u^\mu$  for example, we can express  $\nabla_\mu$  in terms of the partial derivative as

$$\nabla_\mu u^\nu = \partial_\mu u^\nu + \Gamma^\nu{}_{\mu\alpha} u^\alpha, \quad (1.17)$$

where  $\Gamma^\alpha{}_{\mu\nu}$  is an object called the *connection*. The connection does not transform as a type  $(1, 2)$  tensor, which is why it is not referred to as such, but rather is “designed” to transform in a fashion to always cancel the extra terms in the transformation law for the partial derivative of tensors:

$$\Gamma'^\lambda{}_{\epsilon\sigma} = \Lambda^\lambda{}_\alpha (\Lambda^{-1})_\epsilon{}^\mu (\Lambda^{-1})_\sigma{}^\nu \Gamma^\alpha{}_{\mu\nu} - (\Lambda^{-1})_\epsilon{}^\mu (\Lambda^{-1})_\sigma{}^\nu \partial_\mu \Lambda^\lambda{}_\nu. \quad (1.18)$$

In general, the covariant derivative applies to a type  $(n, m)$  tensor by writing  $nm + 1$  terms, corresponding to one partial derivative term and a set of connection terms, each containing a sum with the connection and each index in turn of the type  $(n, m)$  tensor, where upper indices get a plus sign and lower indices get a minus sign:

$$\begin{aligned} \nabla_\mu T^{\alpha_1 \dots \alpha_n}{}_{\beta_1 \dots \beta_m} &= \partial_\mu T^{\alpha_1 \dots \alpha_n}{}_{\beta_1 \dots \beta_m} + \Gamma^{\alpha_1}{}_{\mu\epsilon} T^{\epsilon \dots \alpha_n}{}_{\beta_1 \dots \beta_m} + \dots + \Gamma^{\alpha_n}{}_{\mu\epsilon} T^{\alpha_1 \dots \epsilon}{}_{\beta_1 \dots \beta_m} \\ &\quad - \Gamma^\epsilon{}_{\mu\beta_1} T^{\alpha_1 \dots \alpha_n}{}_{\epsilon \dots \beta_m} - \dots - \Gamma^\epsilon{}_{\mu\beta_n} T^{\alpha_1 \dots \alpha_n}{}_{\beta_1 \dots \epsilon}. \end{aligned} \quad (1.19)$$

The connection is not uniquely defined by its transformation law, so some additional assumptions need to be made. We now specialize our interest to *Riemannian* connections, defined relative to a *psuedo-Riemannian* manifold, where the connection is demanded to be symmetric and the covariant derivative is demanded to be metric compatible:

$$\Gamma^\alpha{}_{[\mu\nu]} = 0, \quad \nabla_\alpha g_{\mu\nu} = 0. \quad (1.20)$$

This comes directly from Einstein's strong equivalence principle, which states that at any point in a spacetime, a locally Minkowskian frame can always be constructed, which is to say that curved spacetimes under these assumptions are always locally flat at a point, which requires the two properties above. This uniquely defines the connection relative to the metric,

$$\Gamma^\alpha_{\mu\nu} = g^{\alpha\beta}(\partial_{(\mu}g_{\nu)\beta} - \frac{1}{2}\partial_\beta g_{\mu\nu}), \quad (1.21)$$

which under these assumptions is known as the *Christoffel symbols*.

Another important tool we will need is the *Lie derivative*. This operator measures the change in an object along a given trajectory in the spacetime manifold. Suppose a trajectory has tangent vector field  $u^\mu$ , then the Lie derivative ( $\mathcal{L}_u$ ) of the tensor field  $T^{\alpha_1 \dots \alpha_n}_{\beta_1 \dots \beta_m}$  is

$$\begin{aligned} \mathcal{L}_u T^{\alpha_1 \dots \alpha_n}_{\beta_1 \dots \beta_m} &= u^\mu \partial_\mu T^{\alpha_1 \dots \alpha_n}_{\beta_1 \dots \beta_m} - (\partial_\epsilon u^{\alpha_1}) T^{\epsilon \dots \alpha_n}_{\beta_1 \dots \beta_m} - \dots - (\partial_\epsilon u^{\alpha_n}) T^{\alpha_1 \dots \epsilon}_{\beta_1 \dots \beta_m} \\ &\quad + (\partial_{\beta_1} u^\epsilon) T^{\alpha_1 \dots \alpha_n}_{\epsilon \dots \beta_m} + \dots + (\partial_{\beta_n} u^\epsilon) T^{\alpha_1 \dots \alpha_n}_{\beta_1 \dots \epsilon}. \end{aligned} \quad (1.22)$$

The Lie derivative of a type  $(n, m)$  tensor field always produces another type  $(n, m)$  tensor field as a result. Note that this coordinate expression for the Lie derivative is valid *only* for tensor fields, and does not apply to non-tensor objects. An example of a Lie derivative of a non-tensor field is that of the Christoffel symbols, whose Lie derivative is

$$\mathcal{L}_u \Gamma^\alpha_{\mu\nu} = u^\beta \partial_\beta \Gamma^\alpha_{\mu\nu} + 2\Gamma^\alpha_{\beta(\mu} \partial_{\nu)} u^\beta - \Gamma^\beta_{\mu\nu} \partial_\beta u^\alpha + \partial_\mu \partial_\nu u^\alpha. \quad (1.23)$$

Although  $\Gamma^\alpha_{\mu\nu}$  is not a tensor, its Lie derivative is in fact a type  $(1, 2)$  tensor. The Lie derivative introduces the concept of *Lie transport*. Any tensor whose Lie derivative vanishes is said to be Lie transported along the curve  $u^\mu$  is tangent to, which is deeply connected to the symmetries present in a spacetime. If the metric tensor is Lie transported along a vector field  $\xi^\mu$ ,

$$\mathcal{L}_\xi g_{\mu\nu} = 2\nabla_{(\mu} \xi_{\nu)} = 0, \quad (1.24)$$

then  $\xi^\mu$  is called a *Killing vector* and the spacetime is said to admit a Killing symmetry. If a metric is independent of time for example, it contains a timelike Killing vector  $\xi^\mu = \partial_t x^\mu$ . As will be discussed in later chapters, Killing symmetries are intimately connected with conserved quantities.

Next, we introduce the Riemann tensor, a 4 index tensor that measures the spacetime curvature of a manifold. In terms of the Christoffel symbols, it reads

$$R^\alpha_{\beta\mu\nu} = 2\partial_{[\mu} \Gamma^\alpha_{\nu]\beta} + 2\Gamma^\alpha_{\epsilon[\mu} \Gamma^\epsilon_{\nu]\beta}. \quad (1.25)$$

It can be shown to measure the failure of the covariant derivative to commute:

$$2\nabla_{[\mu}\nabla_{\nu]}u_{\alpha} = R^{\beta}_{\alpha\mu\nu}u_{\beta} . \quad (1.26)$$

The Riemann tensor is important as it defines the curvature of a manifold. A metric is flat if and only if its Riemann tensor vanishes. This is clearly the case for the Minkowski metric, but strange coordinate transformations can make a flat metric look arbitrarily complicated, and calculating its Riemann tensor is the only way to verify it is indeed a flat metric. By contracting the Riemann tensor, we obtain the Ricci tensor:

$$R_{\mu\nu} = R^{\beta}_{\alpha\beta\nu} . \quad (1.27)$$

To develop Einstein's theory of gravity, we start by considering the stress energy tensor  $T_{\mu\nu}$ , which describes the energy, momentum, and stress of matter fields on the manifold, which satisfies an important property that it is divergenceless:  $\nabla^{\mu}T_{\mu\nu} = 0$ . A consistent theory of gravity will relate the matter fields to the curvature of spacetime, but the tensor that describes the curvature must also be divergenceless. Einstein introduced the Einstein tensor

$$G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = 0 , \quad (1.28)$$

that satisfies  $\nabla^{\mu}G_{\mu\nu} = 0$ , which is known as the contracted Bianchi identity. In fact, by Lovelock's theorem,  $G_{\mu\nu}$  is the only symmetric tensor combination of first and second derivatives of the metric that satisfies this property on a four dimensional manifold. Einstein's field equations can then be cast as a simple relation between curvature and matter:

$$G_{\mu\nu} = 8\pi T_{\mu\nu} . \quad (1.29)$$

From the perspective of numerical relativity, where these field equations are solved using finite arithmetic on a computer, it is sometimes more convenient to start from the "trace reversed form"

$$R_{\mu\nu} = 8\pi(T_{\mu\nu} - \frac{1}{2}g_{\mu\nu}T) , \quad (1.30)$$

where  $T = g^{\mu\nu}T_{\mu\nu}$ . These ten equations represent the evolution of the metric on a spacetime manifold given the matter content within that manifold. From here, figuring out how to write these equations in a form that can readily be numerically integrated on a computer is still a non-trivial task.

### 1.2.3 Manifold Projections

Now that we have the ability to define a spacetime metric  $g_{\mu\nu}$  as a solution to the Einstein field equations, we will refer to the four dimensional manifold on which this solution resides  $\mathcal{M}$ . There are several sub-manifolds within this spacetime that are important to introduce.

First, we consider the  $3 + 1$  projection. This divides the four dimensional spacetime into one timelike direction and a series of spacelike three dimensional hypersurfaces. Given our metric and coordinate vector  $x^\mu$ , we pick out a family of hypersurfaces of constant time  $\mathcal{N}_t$ , for any time  $t_0$ . These hypersurfaces are parameterized by a function:

$$\Phi(x^\mu) = t - t_0 = 0. \quad (1.31)$$

The unit normal covector to these hypersurfaces is defined by the gradient of this function

$$n_\mu = (-\alpha, 0, 0, 0) \propto \nabla_\mu \Phi, \quad (1.32)$$

where  $\alpha$  is called the *lapse*, which acts to ensure that  $n_\mu$  is a unit timelike vector

$$g^{\mu\nu} n_\mu n_\nu = -1, \quad \alpha^2 = (-g^{tt})^{-1}, \quad (1.33)$$

with the sign of the vector chosen such that  $n^\mu$  points into the future. When  $n^\mu$  has its index raised, it has the form

$$n^\mu = (1, -\beta^i)/\alpha, \quad (1.34)$$

where  $\beta^i$  is called the shift. Together, the lapse and shift are four functions that are tied to the four gauge (or coordinate) choice freedoms in the metric. Here and elsewhere, lowercase Latin indices stand for the set of purely spatial coordinates on the constant time slices  $y^i = (x, y, z)$ . Although it seems natural to keep the same coordinates for the spatial directions as we had on the manifold  $\mathcal{M}$ , we are not required to, and  $y^i = (x', y', z')$  could stand for any other set of coordinates we like. We separate  $g_{\mu\nu}$  into temporal parts and spatial parts as

$$g_{\mu\nu} = -n_\mu n_\nu + \gamma_{\mu\nu}, \quad (1.35)$$

where  $\gamma_{\mu\nu}$  is the metric of the three dimensional hypersurface. It still has ten components until we dimensionally project it given our coordinate choice for this hypersurface

$$\gamma_{ij} = \left( \frac{\partial x^\mu}{\partial y^i} \right) \left( \frac{\partial x^\nu}{\partial y^j} \right) \gamma_{\mu\nu}, \quad (1.36)$$

which now only has six components. In numerical relativity, it is common to take the same coordinates for the spatial directions as were used in the four dimensional metric so that the projection is simply

$$\gamma_{ij} = \delta_i^\mu \delta_j^\nu \gamma_{\mu\nu}, \quad (1.37)$$

with this choice not often explicitly stated.

Similarly, we can instead perform a spacelike projection, where a  $2 + 1$  dimensional hypersurface of the original four dimensional spacetime is picked out by a different function

$$\Psi(x^\mu) = 0. \quad (1.38)$$

An example of such a hypersurface would be a time independent coordinate sphere of radius  $R_0$ , parameterized by

$$\Psi(x^\mu) = x^2 + y^2 + z^2 - R_0^2 = 0. \quad (1.39)$$

If all constant time slices of this  $2 + 1$  dimensional hypersurface are closed 2 dimensional surfaces such as a sphere, then the hypersurface is called a “worldtube”. The spacelike unit normal to the hypersurface is given by its normalized gradient:

$$r_\mu = \nabla_\mu \Psi / \psi, \quad (1.40)$$

with the overall sign chosen (by convention) to point out of the manifold  $\mathcal{M}$  and the normalization factor is given by  $\psi^2 = g^{\mu\nu} \nabla_\mu \Psi \nabla_\nu \Psi$ . The vector  $r^\mu$  need not be orthogonal to  $n^\mu$ , as the motion of the worldtube (i.e. the time dynamics of the chosen  $\Psi(x^\mu)$ ) may force it to point into the past or future, as long as the vector itself remains spacelike by assumption. In this example, the spherical surface and its history form the worldtube which we will call  $\mathcal{B}$ . The metric on  $\mathcal{B}$  is related to the four metric as

$$h_{\mu\nu} = g_{\mu\nu} - r_\mu r_\nu. \quad (1.41)$$

Another important quantity is known as the extrinsic curvature. It is a measure of extrinsic aspects of the curvature of a hypersurface, in contrast to  $h_{\mu\nu}$  which is a measure on intrinsic aspects of the hypersurface. The extrinsic curvature of  $\mathcal{B}$  is given by

$$\kappa_{\mu\nu} = h_\mu^\alpha h_\nu^\beta \nabla_\alpha r_\beta = \frac{1}{2} h_\mu^\alpha h_\nu^\beta (\mathcal{L}_r g_{\alpha\beta}), \quad (1.42)$$

or, purely in terms of derivatives of the metric and the function  $\Psi(x^\mu)$ ,

$$\kappa_{\mu\nu} = \frac{1}{2} h_\mu^\alpha h_\nu^\beta \left( r^\lambda \partial_\lambda g_{\alpha\beta} - 2 r^\lambda \partial_{(\alpha} g_{\beta)\lambda} + \frac{2}{\psi} \partial_\alpha \partial_\beta \Psi \right). \quad (1.43)$$

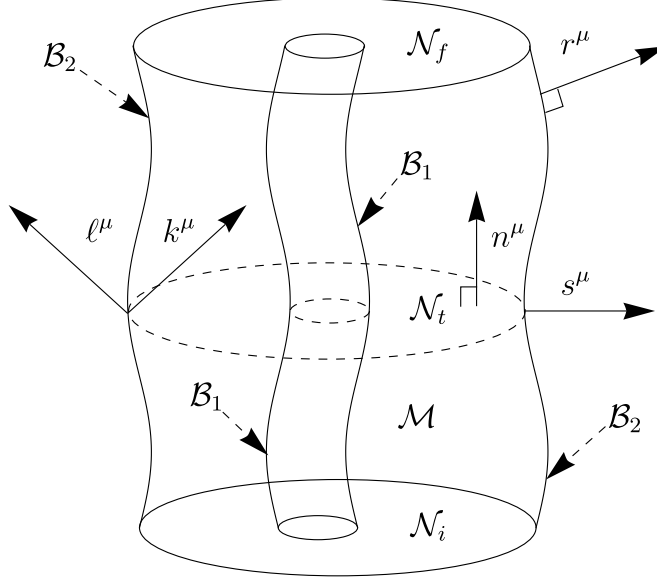


Figure 1.2: Diagram labeling the four dimensional manifold  $\mathcal{M}$  and the various hypersurfaces of interest that bound, foliate, and excise it. Here, time runs on the vertical, the 3-space is horizontal, and null rays run along  $45^\circ$  lines. While  $\mathcal{M}$  is a  $3 + 1$  spacetime,  $\mathcal{N}_t$  is a 3 space, and  $\mathcal{B}_1$  and  $\mathcal{B}_2$  are  $2 + 1$  spacetime worldtubes. The initial and final spatial hypersurfaces  $\mathcal{N}_i$  and  $\mathcal{N}_f$  bound  $\mathcal{M}$  from the past and the future respectively, while  $\mathcal{B}_2$  bounds  $\mathcal{M}$  spatially and  $\mathcal{B}_1$  excises a region interior to  $\mathcal{M}$ .

We can also write the extrinsic curvature of the constant time slices, which simplifies as second derivatives of  $\Phi$  vanish:

$$K_{\mu\nu} = \frac{1}{2} \gamma_\mu^\alpha \gamma_\nu^\beta (n^\lambda \partial_\lambda g_{\alpha\beta} - 2n^\lambda \partial_{(\alpha} g_{\beta)\lambda}) . \quad (1.44)$$

At the boundary worldtube  $\mathcal{B}$ , we introduce the purely spatial normal  $s^\mu \propto \gamma^\mu_\nu r^\nu$  which is normalized to make it a unit vector. Together with the timelike normal  $n^\mu$  orthogonal to  $s^\mu$ , we can define two null or lightlike vectors at the intersection of  $\mathcal{B}$  and  $\mathcal{N}_t$ . Conventions differ in the literature, but we will chose the following definitions here:

$$k^\mu = \frac{1}{\sqrt{2}}(n^\mu - s^\mu), \quad \ell^\mu = \frac{1}{\sqrt{2}}(n^\mu + s^\mu). \quad (1.45)$$

These are the ingoing and outgoing null vectors respectively, and they have the following properties:

$$k^\mu k_\mu = \ell^\mu \ell_\mu = 0, \quad k^\mu \ell_\mu = -1. \quad (1.46)$$

We can re-express  $g_{\mu\nu}$  in terms of these vectors:

$$g_{\mu\nu} = -2k_{(\mu}\ell_{\nu)} + \sigma_{\mu\nu} , \quad (1.47)$$

where  $\sigma_{\mu\nu}$  is the metric for the two dimensional spatial surface of the boundary evaluated at some time slice of the worldtube. Figure 1.2 labels all of the vectors and manifolds that may be typically encountered in a Cauchy evolution based numerical relativity simulation.

### 1.2.4 Black Holes

One of the simplest exact solutions to Einstein's vacuum field equations was first described by Schwarzschild and is known as the Schwarzschild solution. It describes what is now known as a black hole, and in his original orthogonal spherical-like coordinates  $x^\mu = (t, r, \theta, \varphi)$  is given in terms of the line element by

$$ds^2 = -(1 - 2M/r)dt^2 + (1 - 2M/r)^{-1}dr^2 + r^2d\theta^2 + r^2\sin^2(\theta)d\varphi^2 . \quad (1.48)$$

These coordinates turn out to be a poor choice in which to analyze the properties of the Schwarzschild solution, so a coordinate transformation to Kerr-Schild coordinates is useful. This metric is given in terms of the line element in Cartesian-like coordinates  $x^\mu = (t, x, y, z)$  as

$$ds^2 = -dt^2 + dx^2 + dy^2 + dz^2 + \frac{2M}{r}(dt + dr)^2 , \quad (1.49)$$

where  $r^2 = x^2 + y^2 + z^2$ . This spacetime describes a physical object of mass  $M$  and the surrounding spacetime, which is called static as it contains a vector  $\xi^\mu = \partial_t x^\mu$  that in addition to being a Killing vector is also hypersurface orthogonal ( $\nabla_{[\mu}\xi_{\nu]} = 0$ ). If this Killing vector had not been hypersurface orthogonal, like in a spinning black hole for example, the spacetime is instead called stationary. The Schwarzschild spacetime has some interesting properties at  $r = 2M$ , called the Schwarzschild radius. The surface  $r = 2M$  is called the horizon of the black hole, and is unambiguously defined in this spacetime. However, once the spacetime becomes dynamical, there will be several different notions of what “horizon” means.

The surface  $r = 2M$  is where the norm of the Killing vector  $\xi^\mu\xi_\mu = (1 - 2M/r)$  changes sign, turning from timelike on the outside, to spacelike on the inside. This motivates the term *Killing horizon* for this surface. Unfortunately, it has no utility in a dynamical spacetime that may not contain any Killing vectors.

Given a two dimensional surface, we can always define the ingoing and outgoing null vectors  $k^\mu$  and  $\ell^\mu$  on that surface. Considering a set of spherical surfaces surrounding the black hole spacetime, we construct these vectors with  $s^\mu$  pointing radially out from the black hole. The expansion of these null vectors is defined as their divergence:  $\theta_\ell = \nabla^\mu \ell_\mu$ ,  $\theta_k = \nabla^\mu k_\mu$ , and the sign of the expansion dictates whether the null vectors are diverging apart (positive) or converging together (negative). For spheres within the surface  $r = 2M$ , we have  $\theta_\ell < 0$  and  $\theta_k < 0$ , meaning all null vectors are converging toward the origin, and thus these spheres are called *trapped surfaces*. Once the sphere grows to  $r = 2M$ , we find instead  $\theta_\ell = 0$ , which defines this surface as an *apparent horizon*. In principle, an apparent horizon can be found in a dynamical spacetime by looking for a surface where the expansion of  $\ell^\mu$  vanishes.

A more strict definition of a horizon has to do with the null information that can ultimately reach infinitely far away from the black hole. Imagine every point in a spacetime emits a light ray radially away from the black hole. The surface that separates all light rays that reach null infinity, and those that fall back into the black hole, is called the *event horizon*, which is always outside of the apparent horizon. The event horizon has less utility in a dynamical spacetime where information about the future may not yet be available, like in numerical relativity, as the event horizon can only be known once the entire spacetime is completely determined.

### 1.3 Hyperbolicity

In order to solve a system of partial differential equations (called the problem), such as Einstein's field equations, we have to gain an understanding as to what kinds of partial differential systems are solvable in a stable fashion. This is where the concept of well-posedness becomes helpful. A problem is called well-posed when [25, 26, 27]

- At least one solution to the problem exists
- The set of solutions to the problem are unique
- The set of solutions to the problem depend smoothly on the initial conditions

An essential step in proving that a given problem is well posed is writing it in a hyperbolic form. Consider the generic system of evolution equations:

$$\partial_t U_A = [A(U)^B_A]^i \partial_i U_B + S_A(U). \quad (1.50)$$

This system is known as a first-order quasi-linear partial differential system of equations. Here,  $U_A$  is known as the state vector, and it contains all of the evolved fields in the system (which can be quite numerous), and capital Latin indices run over these fields. The index  $i$  runs over the spatial coordinates chosen for the evolution. Here,  $S_A(U)$  are the source terms which depend on  $U_A$ , but not its derivatives. The matrices  $[A(U)^B_A]^i$  are known as the characteristic matrices, which may also depend on  $U_A$ , but not its derivatives. The structure of the characteristic matrices define the concept of hyperbolicity [25, 26, 27], where for any unit vector  $s_i$ :

- **Weak hyperbolicity:** The matrix  $s_i [A(U)^B_A]^i$  has strictly real eigenvalues.
- **Strong hyperbolicity:** The system is weakly hyperbolic and the matrix  $s_i [A(U)^B_A]^i$  is diagonalizable.
- **Symmetric hyperbolicity:** The system is strongly hyperbolic and there exists a symmetric positive definite matrix  $\mathcal{S}^B_A$  called the symmetrizer, that does not depend on  $s_i$ , such that  $s_i \mathcal{S}^B_C [A(U)^C_A]^i$  is a Hermitian matrix.

The eigenvectors of  $s_i [A(U)^B_A]^i$  define the *characteristic modes* and the eigenvalues define the *characteristic speeds*<sup>1</sup> of the system relative to the unit vector  $s_i$ . The characteristic modes separate the statevector into parts that propagate in distinct directions with distinct speeds, which is useful for applying boundary conditions.

The best systems are those that can be cast as symmetric hyperbolic, as they are guaranteed to be well-posed if the characteristic matrices are independent of  $U_A$ . This will not be the case in general, but for many of the formulations of Einstein’s equations considered in this work, independence of  $U_A$  is a good approximation in weak gravity regions. Symmetric hyperbolicity also comes with the concept of an energy estimate, which allows for proofs of energy stability.

The energy density estimate of a symmetric hyperbolic system is defined via a quadratic form based on a symmetrizer for the system [27]

$$\rho = U^A \mathcal{S}_{AB} U^B, \quad (1.51)$$

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<sup>1</sup>The use of the term “characteristic speeds” is potentially confusing, as it is a signed quantity. The unit vector  $s_i$  defines the sign of these “speeds”, where a positive speed indicates propagation of a characteristic mode *along*  $s_i$  and a negative speed indicates propagation of a characteristic mode in the direction *opposite*  $s_i$ . Characteristic velocity is unfortunately not the term used in the community.

which has corresponding flux density

$$\varphi^i = U^A \mathcal{S}_{AC} [A(U)^C_B]^i U^B. \quad (1.52)$$

The symmetrizer is not unique in general, so there may be a family of them from which to choose. This choice of symmetrizer is arbitrary, and in later chapters we will choose one motivated by examples of energy conservation in stationary spacetimes. The energy density estimate is conserved when  $[A^B_A]^i$  is approximately independent of  $U_A$  and  $S_A(U_B)$  can be approximately neglected (e.g. when we consider small high-frequency perturbations):

$$\partial_t \int \rho dV \sim \oint s_i \varphi^i dS. \quad (1.53)$$

Numerical instability tends to occur when high frequency numerical noise grows without bound. A symmetric hyperbolic system ensures that due to the conservation of the energy estimate, this high frequency noise cannot grow without bound in principle.

## 1.4 Numerical Methods

Solutions to the generic system of evolution equations Eq. (1.50) can be arbitrarily complicated and only in a small class of simple cases can one hope to find an exact solution. Instead, an approximate numerical solution is sought, where the problem is discretized in both time and space. The list of numerical techniques one might apply to achieve this is long, but for the scope of this thesis, only finite differencing techniques for approximations to spatial derivatives, and Runge-Kutta techniques for discrete time advancement will be introduced.

### 1.4.1 Finite Differencing

The first step in approximating the system Eq. (1.50) is defining a way to approximate spatial derivatives using a finite representation of the functions of which the spatial derivative is needed. One of the many ways to approximate spatial derivatives is the method of finite differencing.

Consider a function  $f(x)$  that is represented by grid points equally spaced by a distance  $h$  within a domain  $x \in (a, b)$ , where  $a < b$ . Using a finite number of points, we require a

consistent approximation of the partial derivative. As is usually introduced in continuous calculus, the definition of the derivative is written

$$\partial_x f(x) = \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h}. \quad (1.54)$$

If the limit is neglected, this becomes a consistent approximation to the derivative using only two sampled points of the function  $f(x)$ . If we consider the series expansion of  $f(x+h)$  in terms of  $h$ , we obtain

$$f(x+h) = f(x) + \partial_x f(x)h + \frac{1}{2}\partial_x^2 f(x)h^2 + \mathcal{O}(h^3), \quad (1.55)$$

which shows that this approximation to the partial derivative gives the correct answer with the first correcting term of order  $h^1$ :

$$\frac{-f(x) + f(x+h)}{h} = \partial_x f(x) + \frac{1}{2}\partial_x^2 f(x)h + \mathcal{O}(h^2). \quad (1.56)$$

Since the error in the approximation is dominated by a term  $\mathcal{O}(h^1)$ , this approximation is called first order accurate. This approximation scheme includes one function evaluation point at  $x$ , and one farther along at  $x+h$ , so it is called a *forward differencing* scheme. We can define a *backward differencing* scheme by instead considering the backward expansion

$$f(x-h) = f(x) - \partial_x f(x)h + \frac{1}{2}\partial_x^2 f(x)h^2 + \mathcal{O}(h^3), \quad (1.57)$$

and manipulating it to reveal the partial derivative as before:

$$\frac{-f(x-h) + f(x)}{h} = \partial_x f(x) - \frac{1}{2}\partial_x^2 f(x)h + \mathcal{O}(h^2), \quad (1.58)$$

which shows the same first order accuracy as the forward case. We can take Eq. (1.56) and add it to Eq. (1.58) to obtain a more accurate approximation to the derivative:

$$\frac{-f(x-h) + f(x+h)}{2h} = \partial_x f(x) + \frac{1}{6}\partial_x^3 f(x)h^2 + \mathcal{O}(h^4). \quad (1.59)$$

This is called a *centered differencing* scheme, and since the error is now dominated by terms  $\mathcal{O}(h^2)$ , it is called second order accurate. If we instead subtract Eq. (1.56) and Eq. (1.58), we obtain an approximation for the second derivative:

$$\frac{f(x-h) - 2f(x) + f(x+h)}{h^2} = \partial_x^2 f(x) + \frac{1}{12}\partial_x^4 f(x)h^2 + \mathcal{O}(h^4), \quad (1.60)$$

which is also second order accurate.

In general, by including more function evaluation points with which to approximate the derivative, higher order accuracy schemes can be derived. As they will be used in later chapters of this thesis, the fourth order accurate centered scheme

$$\frac{f(x-2h) - 8f(x-h) + 8f(x+h) - f(x+2h)}{12h} = \partial_x f(x) + \frac{1}{30} \partial_x^5 f(x) h^4 + \mathcal{O}(h^6), \quad (1.61)$$

and the sixth order accurate centered scheme

$$\begin{aligned} & \frac{-f(x-3h) + 9f(x-2h) - 45f(x-h) + 45f(x+h) - 9f(x+2h) + f(x+3h)}{60h} \\ &= \partial_x f(x) + \frac{1}{140} \partial_x^7 f(x) h^6 + \mathcal{O}(h^8), \end{aligned} \quad (1.62)$$

are defined. Centered schemes are useful in the interior of the domain, where there are enough grid points in either direction to calculate the desired accuracy of finite differencing stencil. When the derivative is required near the boundaries of the domain however, a centered scheme will not be possible. One way to circumvent this problem is to introduce forward differencing schemes near the left boundary ( $x = a$ ) and backward differencing schemes near the right boundary ( $x = b$ ). Unfortunately, this tends to lead to numerically unstable evolution of the system unless great care is taken in how the transition between centered and forward/backward schemes is made. This is where the next concept of summation by parts becomes helpful.

### 1.4.2 Summation by Parts

As first introduced and defined in [28], and reviewed in [29], summation by parts derivative operators provide a means to prove the stability of discrete problems via the energy method. This method proves the numerical stability of a problem by showing that there exists a numerical energy, that depends on the entire solution domain and the entire state vector, that is bounded and thus the system cannot be numerically unstable or else this quantity would by definition be unbounded.

To see how summation by parts works, we will analyze the one dimensional flat wave equation in Cartesian coordinates as an example:

$$(-\partial_t^2 + \partial_x^2)\phi = 0. \quad (1.63)$$

If we define auxiliary variables to hold the time derivative  $u = -\partial_t \phi$  and the spatial derivative  $v_x = \partial_x \phi$ , then we can write a system of evolution equations that contains only first derivatives

$$\begin{aligned}\partial_t \phi &= -u, \\ \partial_t v_x + \partial_x u &= 0, \\ \partial_t u + \partial_x v_x &= 0,\end{aligned}\tag{1.64}$$

Where the first equation is just a definition, the second enforces the commutativity of temporal and spatial derivatives, and the third is the wave equation. If we consider the spatial domain  $x \in [a, b]$ , the wave equation has an energy conservation law due to its propagation on a static background spacetime:

$$\partial_t \int_a^b \frac{1}{2}(u^2 + v_x^2) dx = uv_x \Big|_a^b.\tag{1.65}$$

Distributing the time derivative into the energy and substituting the evolution equations yields an integration by parts rule

$$\int_a^b u \partial_x v_x dx + \int_a^b (\partial_x u) v_x dx = uv_x \Big|_a^b.\tag{1.66}$$

If this integration by parts rule was violated, then the wave equation system would not have a conserved energy, and could then potentially be an analytically unstable system of equations. Integration by parts is always obeyed because it is a fundamental theorem in continuous calculus, but once we make the jump to finite calculus (i.e. finite differencing), this is no longer guaranteed. Instead, finite differencing operators have to be specially designed to obey a discrete analog of integration by parts, which is the basis for summation by parts.

Consider the system now sampled on a grid. The domain is discretized with  $n$  grid points from  $x = a$  to  $x = b$  with a constant grid spacing  $h = (b - a)/(n - 1)$ . The functions  $\phi$ ,  $u$ , and  $v_x$  are now represented by vectors of  $n$  points and the spatial derivatives are approximated with an  $n \times n$  finite differencing operator  $D_x$ :

$$\begin{aligned}\partial_t \phi &= -u, \\ \partial_t v_x + D_x u &= 0, \\ \partial_t u + D_x v_x &= 0.\end{aligned}\tag{1.67}$$

A summation by parts operator  $D_x$  and its corresponding  $n \times n$  symmetric and positive definite norm operator  $\Sigma$  satisfy the following property:

$$\Sigma D_x + D_x^T \Sigma = B, \quad (1.68)$$

where  $B = \text{diag}(-1, 0, \dots, 0, 1)$  is the  $n \times n$  boundary operator. Multiplying  $u$  on the left and  $v_x$  on the right, we obtain

$$u^T \Sigma D_x v_x + (D_x u)^T \Sigma v_x = u^T B v_x = u(b)v_x(b) - u(a)v_x(a). \quad (1.69)$$

This property directly mimics the continuous integration by parts. We can see that if we apply for example  $u(a) = 0$  and  $v_x(b) = 0$  as boundary conditions, the summation by parts property assures that the numerical energy estimate  $E_n$  is conserved even on a discrete grid:

$$\partial_t E_n \equiv \partial_t \left( \frac{1}{2} u^T \Sigma u + \frac{1}{2} (v_x)^T \Sigma v_x \right) = 0. \quad (1.70)$$

For a given set of arbitrary boundary conditions, if the numerical energy  $E_n$  can be shown to be strictly decreasing

$$\partial_t E_n \leq 0, \quad (1.71)$$

for all time, then the problem is called *energy stable*. The property of energy stability proves that the semi-discrete problem is numerically stable, that is when time derivatives are taken to be exact. In a realistic scenario, time advancement will be discrete as well, so the numerical stability of the problem will also depend on the time discretization scheme chosen. How the boundary conditions are applied is also important, as numerical tests tend to show that applying a boundary condition exactly (i.e. replacing  $u$  and/or  $v_x$  with exact values) tends to make the numerical problem stiff at the boundary and can lead to instability. To combat this problem, another concept called simultaneous approximation terms is introduced.

### 1.4.3 Simultaneous Approximation Terms

One way to apply boundary conditions in numerical systems is to use simultaneous approximation terms, which have been shown to be a successful way to keep a system energy stable. At the boundary points, an exponential decay term is added to the evolution equations that will evolve the state vector toward the desired boundary values at a given decay

timescale. We define  $e_a = (1, \dots, 0)$  and  $e_b = (0, \dots, 1)$  to select the grid points at  $x = a$  and  $x = b$  respectively, and write the following numerical scheme:

$$\begin{aligned}\partial_t \phi &= -u, \\ \partial_t v_x + D_x u &= \tau \Sigma^{-1} e_a (v_x^{\text{BC1}} - v_x) + \tau \Sigma^{-1} e_b (v_x^{\text{BC2}} - v_x), \\ \partial_t u + D_x v_x &= \tau \Sigma^{-1} e_a (u^{\text{BC1}} - u) + \tau \Sigma^{-1} e_b (u^{\text{BC2}} - u),\end{aligned}\tag{1.72}$$

where  $u^{\text{BC}(1,2)}$  and  $v_x^{\text{BC}(1,2)}$  are the boundary conditions to be applied at  $x = a$  and  $x = b$  respectively, and  $\tau$  controls the exponential decay scale toward these desired boundary values. To show energy stability, we take the time derivative of  $E_n$

$$\partial_t E_n = \frac{1}{2} \partial_t (u^T \Sigma u + (v_x)^T \Sigma v_x) = u^T \Sigma \partial_t u + (\partial_t v_x)^T \Sigma v_x,\tag{1.73}$$

and substitute in the evolution equations and the summation by parts property

$$\begin{aligned}\partial_t E_n &= u(a) s^x(a) v_x(a) + u(a) u^{\text{BC1}} - u(a)^2 + v_x(a) v_x^{\text{BC1}} - v_x(a)^2 \\ &\quad + u(b) s^x(b) v_x(b) + u(b) u^{\text{BC2}} - u(b)^2 + v_x(b) v_x^{\text{BC2}} - v_x(b)^2.\end{aligned}\tag{1.74}$$

Here, at the boundary points, the unit normal vector  $s^\mu$  to the boundary is defined to point out of the domain, and in one dimension has only one component  $s^x$ . Since this system is propagating on a flat background spacetime, we have  $s^x(a) = -1$ ,  $s^x(b) = 1$ , and  $s^x = s_x$ . Relative to  $s^\mu$ , we define the characteristic modes for this system by calculating the eigenvectors of the characteristic matrices. In this case, there are two modes only<sup>2</sup>:

$$U^- = \ell^\mu \partial_\mu \phi = -\frac{1}{\sqrt{2}}(u + s^x v_x), \quad U^+ = k^\mu \partial_\mu \phi = -\frac{1}{\sqrt{2}}(u - s^x v_x).\tag{1.75}$$

These characteristic modes  $U^\pm$  have characteristic speeds  $c_\pm = \pm 1$  respectively. The generic way to apply boundary conditions to systems of hyperbolic equations is to provide boundary conditions for every characteristic mode that is propagating into the domain, i.e. ones that have a negative characteristic speed. To do this, we write the state vector in terms of the characteristic modes:

$$u = -\frac{1}{\sqrt{2}}(U^+ + U^-), \quad v_x = -\frac{1}{\sqrt{2}}s_x(U^- - U^+).\tag{1.76}$$

The boundary condition values  $u^{\text{BC}}$  and  $v_x^{\text{BC}}$  are obtained by making the substitution  $U^- \rightarrow U^{-\text{BC}}$  in the above definitions for each of the boundaries, since these are the only

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<sup>2</sup>In Chapter 2, the characteristic modes are defined differently, with an  $s^\mu$  pointing in the positive radial direction since the problem being solved is spherically symmetric.

characteristic modes with negative characteristic speed in this case. We then consider the following family of boundary conditions

$$U^{-\text{BC}} = kU^+, \quad (1.77)$$

for any scalar  $k$ , which are motivated by the control of the energy flux at each boundary. Finally, in terms of the characteristic modes, we have

$$\begin{aligned} \partial_t E_n = & \left[ -\frac{1}{2}(U^- - U^+)^2 - (1 - k\tau)U^+U^- - (\tau - 1)(U^-)^2 \right] |_a \\ & + \left[ -\frac{1}{2}(U^- - U^+)^2 - (1 - k\tau)U^+U^- - (\tau - 1)(U^-)^2 \right] |_b. \end{aligned} \quad (1.78)$$

We are interested in the values of the parameters  $\tau$  and  $k$  for which the energy is strictly decreasing for all time. Although for homogeneous boundary conditions ( $k = 0$ ), the scheme is energy stable for all  $\tau > \frac{1}{2}$ , we require a scheme that is stable for a range of boundary condition choices. Taking  $\tau = 1$  we have

$$\begin{aligned} \partial_t E_n = & \left[ -\frac{1}{2}(U^+ - kU^-)^2 + \frac{1}{2}(k^2 - 1)(U^-)^2 \right] |_a \\ & + \left[ -\frac{1}{2}(U^+ - kU^-)^2 + \frac{1}{2}(k^2 - 1)(U^-)^2 \right] |_b, \end{aligned} \quad (1.79)$$

which is energy stable if  $-1 \leq k \leq 1$ . This directly mimics the continuous case, as the set of boundary conditions  $-1 \leq k \leq 1$  include those that are perfectly reflecting ( $k = \pm 1$ ) and perfectly transmitting ( $k = 0$ ), which has the energy either preserved or decreasing in all cases. There is nothing wrong with having  $|k| > 1$  in principle, as in the continuous problem this just means that more energy is injected into the system than is incident on the boundary from within the domain, but the system is then not energy stable even in the continuum as this can lead to a feedback loop of injected energy, which can grow without bound. As long as  $|k| \leq 1$  the continuous problem is energy stable and as long as  $\tau = 1$ , the numerical problem is also energy stable.

Simple one dimensional problems like the one considered here have fairly simple energy stability requirements, but more complicated equations, like those that have characteristic speeds that are functions of space and time, will have more complicated energy stability requirements. It is shown in [30] that  $\tau$  should be set to the magnitude of the incoming characteristic speed  $|c_-|$  in such cases, making the boundary conditions more weakly applied the closer the boundary is to a null surface, like if it was placed close to the horizon of a black hole.

#### 1.4.4 Runge-Kutta methods

Next, we introduce a family of numerical time advancement methods. The generic system of Eq. (1.50) can be rewritten in terms of a set of functions  $f_A$  that depend only on the

state vector  $U_A$  and its first spatial derivatives:

$$\partial_t U_A = f_A(\partial_i U_B, U_B). \quad (1.80)$$

When the substitution  $\partial_i \rightarrow D_i$  is made with an appropriate set of SBP operators  $D_i$  and BCs are applied using SATs, the entirety of  $f_A$  can be approximated on a grid. Now, a numerical method of time advancement needs to be introduced to advance the current solution to the next time slice given the values of  $\partial_t U_A$  that can now be calculated. To show how this is done, the notation will be adjusted with vector hats  $U_A \rightarrow \vec{U}$ .

A popular set of methods are the explicit Runge-Kutta methods, which are a class of time discretization methods that can be derived to various orders of accuracy. A fundamental example of a Runge-Kutta method is the forward Euler method. To explain how this method would work on a computer, we will introduce the variable assignment operator  $\leftarrow$  which indicates the writing the value of the right hand side into the variable on the left hand side (normally '=' in most computer languages).

Given an initial value for the whole state vector  $\vec{U}(t = 0)$ , we allocate two computer memory registers to hold information about the state vector and call them  $\vec{U}_{1,2}$ . We store the initial values in  $\vec{U}_1$ :  $\vec{U}_1 \leftarrow \vec{U}(t = 0)$ , and then each subsequent time step by interval  $\Delta t$  involves one stage, first performing the forward Euler step and storing it in  $\vec{U}_2$ , then copying back into  $\vec{U}_1$ :

$$\begin{aligned} \vec{U}_2 &\leftarrow \vec{U}_1 + \vec{f}(\vec{U}_1) \Delta t, \\ \vec{U}_1 &\leftarrow \vec{U}_2. \end{aligned} \quad (1.81)$$

The forward Euler algorithm, although only first order accurate, is very memory efficient, as it only ever needs two memory registers. In principle the scheme

$$\vec{U}_1 \leftarrow \vec{U}_1 + \vec{f}(\vec{U}_1) \Delta t, \quad (1.82)$$

is possible as well, but since  $\vec{f}(\vec{U}_1)$  contains finite differencing operators, it depends on many other grid points in the vicinity of whatever grid point is currently being calculated. This runs the risk of points being overwritten before an adjacent point can be calculated which may need the value that was just overwritten. Although clever methods to prevent this issue exist, we will assume this is not possible, which will better allow for computer parallelization over grid points. As a result, assignments of the form  $\vec{U}_1 \leftarrow \vec{f}(\vec{U}_1)$  will be forbidden. Unfortunately, this means Runge-Kutta methods more accurate than the forward Euler will require even more memory be allocated.

Another time stepping algorithm used in this thesis is the so-called strong stability preserving third order Runge-Kutta method (RK3) [31]. It requires three separate memory registers ( $\vec{U}_1, \vec{U}_2, \vec{U}_3$ ). The algorithm begins by storing the initial values as before  $\vec{U}_1 \leftarrow \vec{U}(t=0)$ , while  $\vec{U}_2$  and  $\vec{U}_3$  can be initially undefined. It works in the following three stages:

Stage 1:

$$\vec{U}_2 \leftarrow \vec{U}_1 + f(\vec{U}_1)\Delta t,$$

Stage 2:

$$\vec{U}_3 \leftarrow \frac{3}{4}\vec{U}_1 + \frac{1}{4}\vec{U}_2 + \frac{1}{4}\vec{f}(\vec{U}_2)\Delta t,$$

Stage 3:

$$\vec{U}_1 \leftarrow \frac{1}{3}\vec{U}_1 + \frac{2}{3}\vec{U}_2 + \frac{2}{3}\vec{f}(\vec{U}_3)\Delta t,$$

with the result advanced by  $\Delta t$  and stored in  $\vec{U}_1$  for the next integration step.

The reason the number of memory registers used in the time stepping algorithm is of concern is that the memory cost of the evolutions in numerical relativity can be a limiting factor. Consider a three dimensional simulation represented on a grid of  $1000^3$  points. For the generalized harmonic formulation introduced in the next chapter, we require 50 evolved fields in the state vector, and the RK3 algorithm requires 3 state vector memory registers. If each evolved field is represented by a standard 8 byte floating point number, the total allocated system memory required is 1.2 terabytes. This is an uncommonly large amount of system memory for one computer to have<sup>3</sup>, so keeping the number of memory registers low can make the difference between a simulation that is possible or not.

Runge-Kutta methods of higher order accuracy than those presented here exist, but with select summation by parts operators, a high order accuracy time stepping scheme doesn't always make sense. If one restricts to summation by parts operators with diagonal norms with accuracy order  $2p$  in the interior, then the global accuracy is only order  $p+1$  due to decreased accuracy near the boundary points [29]. For example, for a summation by

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<sup>3</sup>At least at the time of this thesis. Of course, supercomputer clusters can have many computer nodes with a total system memory of all computer nodes being much higher than this. Methods other than finite differencing, such as spectral methods, can be much more memory efficient, but come with their own drawbacks.

parts operator based on a fourth order accurate centered scheme in the interior, the global accuracy achieved is only third order, so for this case it doesn't help to pick a Runge-Kutta scheme more accurate than third order.

Lastly, a value for the time step  $\Delta t$  needs to be chosen. In the context of the one dimensional wave system Eqns. (1.72), the time step size is bounded by the so-called CFL stability criterion:

$$C^{CFL} = |c_{\pm}| \frac{\Delta t}{\Delta x} \leq C_{\max}^{CFL}, \quad (1.83)$$

where  $C^{CFL}$  is called the Courant number. The value of the maximum allowed Courant number  $C_{\max}^{CFL}$  to maintain numerical stability depends on the numerical scheme and the system being solved, but is usually of order unity. Some of the more complicated schemes considered in the following chapters have somewhat more strict  $C_{\max}^{CFL}$  bounds.

## 1.5 Symmetric Hyperbolic Formulations of Numerical Relativity

In order to numerically solve Einstein's equations, one must first write down a *formulation* of these equations. This is to say that Einstein's equations as normally written are not necessarily in a form that can be readily numerically integrated in a stable fashion. Even if one casts Einstein's equations in a form that can be integrated, it is not guaranteed that such a system is stable over time. This is why great care is taken to demonstrate formulations that are at least strongly hyperbolic, where well-posedness can be demonstrated. There are many strongly hyperbolic formulations used with relative success over the years, but the best formulations are those that are symmetric hyperbolic. There are a few proposed formulations that are symmetric hyperbolic (see [32, 33, 34, 35, 36] for some examples). Many of these proposed formulations require gauge fixing, making them of less general use. That is to say that symmetric hyperbolicity is ensured in part by assuming some type of coordinate system for all time, preventing a different coordinate choice from being made without losing this property. There do exist some formulations that allow complete gauge freedom however, and we will consider formulations of this type exclusively. Another useful feature not present in every symmetric hyperbolic formulation is the existence of causal characteristic speeds (i.e. ones that lead to propagation exclusively on or within the light-cone). Thus as a starting point for a numerically stable system, we desire a formulation that has the following properties:

- Symmetric Hyperbolicity
- No gauge fixing required
- Causal characteristic speeds

In this thesis, two formulations fitting these requirements are demonstrated. The first formulation used is the so-called Einstein-Christoffel formulation that is demonstrated in spherical symmetry in Chapter 2. The second formulation is the so-called generalized harmonic formulation, demonstrated without symmetry assumptions in Chapter 3. The main difference between these two systems is how the coordinate gauge choices are enforced. The Einstein Christoffel formulation fixes the gauge by specifying four functions of space-time that effectively become the lapse and the shift. The generalized harmonic formulation works instead by specifying four functions that dictate the time evolution of the lapse and shift.

### 1.5.1 The Einstein-Christoffel Formulation

One such formulation that fits all of our requirements is the Einstein-Christoffel formulation, proposed in [33] and refined and numerically tested in [37]. This formulation is implemented using what we will refer to as a “zeroth order gauge” specification. That is to say that in order to choose the gauge under which the spacetime will evolve, a user would specify four functions of spacetime that effectively dictate the values of the lapse and shift at every point in spacetime. One important detail however is that the densitized lapse  $\tilde{\alpha} \equiv \alpha/\sqrt{\gamma}$  is specified, rather than the lapse itself:

$$\tilde{\alpha} = \tilde{\alpha}(x^\mu), \quad \beta^i = \beta^i(x^\mu). \quad (1.84)$$

The dynamical variables will represent the 3-metric  $\gamma_{ij}$  and its derivatives, with the Christoffel symbols with respect to  $\gamma_{ij}$  denoted  $\bar{\Gamma}_{kij}$  with covariant derivative  $\bar{\nabla}_i$ . The functions

$$f_{kij} \equiv \bar{\Gamma}_{(ij)k} + \gamma_{ki}\gamma^{lm}\bar{\Gamma}_{[lj]m} + \gamma_{kj}\gamma^{lm}\bar{\Gamma}_{[li]m}, \quad (1.85)$$

are defined to hold information about the spatial derivatives of  $\gamma_{ij}$ , which can be recovered using the inversion relation

$$\partial_k \gamma_{ij} = 2f_{kij} - 4\gamma^{lm}(f_{lm(i}\gamma_{j)k} - \gamma_{k(i}f_{j)lm}). \quad (1.86)$$

The extrinsic curvature <sup>4</sup>

$$K_{ij} \equiv -\gamma_i^\mu \gamma_j^\nu \nabla_\mu n_\nu = -\frac{1}{2\alpha}(\partial_t - \mathcal{L}_\beta)\gamma_{ij} = -\frac{1}{2\alpha}(\partial_t \gamma_{ij} - \beta^k \partial_k \gamma_{ij} - 2\gamma_{k(i} \partial_{j)} \beta^k), \quad (1.87)$$

is defined to hold information about the time derivatives. The complete state vector for this system can then be written  $\vec{U} = (\gamma_{ij}, f_{kij}, K_{ij})$ , which is a total of 30 evolved fields. Before we can write down the evolution equations, we need to recognize the existence of the constraints in this system. The Hamiltonian constraint is

$$\mathcal{C} \equiv \gamma^{ij} \gamma^{kl} \{2(\partial_k f_{ijl} - \partial_i f_{jkl}) + K_{ik} K_{jl} - K_{ij} K_{kl} + \gamma^{mn} [f_{ikm}(5f_{jln} - 6f_{ljn}) + 13f_{ikl} f_{jmn} + f_{ijk}(8f_{mln} - 20f_{lmn})]\} + 16\pi\rho, \quad (1.88)$$

where  $\rho = T^{\mu\nu} n_\mu n_\nu$  is the energy density of matter fields. The set of momentum constraints are

$$\mathcal{C}_i \equiv \gamma^{kl} \{\partial_i K_{kl} - \partial_k K_{il} + \gamma^{mn} [K_{ik}(3f_{lmn} - 2f_{mnl}) - K_{km} f_{iln}]\} + 8\pi S_i, \quad (1.89)$$

where  $S_i \equiv \gamma_i^\mu n^\nu T_{\mu\nu}$  is the momentum density of matter fields. The rest of the components of the stress energy tensor are given by the spatial stress  $S_{ij} \equiv \gamma_i^\mu \gamma_j^\nu T_{\mu\nu}$ . Finally, by defining  $f_{kij}$ , we introduce a set of spatial derivative constraints

$$\mathcal{C}_{kij} \equiv \partial_k \gamma_{ij} - 2f_{kij} + 4\gamma^{lm} (f_{lm(i} \gamma_{j)k} - \gamma_{k(i} f_{j)lm}). \quad (1.90)$$

Analytically, all of these constraints vanish and are preserved in the evolution, but when spatial derivatives are approximated using finite differencing for example, they will become violated due to numerical error. As long as all of the constraints converge to zero with increasing resolution, the evolution is properly approximating the Einstein field equations.

We then proceed to write an evolution equation for each of the fields in the state vector. The evolution of  $K_{ij}$  is dictated by the Einstein field equations and the evolution of  $\gamma_{ij}$  is dictated by the definition Eq. (1.87). In order to evolve  $f_{kij}$ , a commutation property is enforced:

$$[\partial_t - \mathcal{L}_\beta, \partial_k] = 0, \quad (1.91)$$

which allows us to write an identity for the evolution of the spatial derivatives of the metric

$$(\partial_t - \mathcal{L}_\beta) \partial_k \gamma_{ij} = -\partial_k (2\alpha K_{ij}). \quad (1.92)$$

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<sup>4</sup>Notice that this definition of the extrinsic curvature is different by a minus sign compared to the usual definition Eq. (1.44). This is a common convention in numerical relativity, but is different than that given in [22] for example. It is projected onto the 3-space with  $\delta_i^\mu$  as the coordinates on the 3-space  $y^i$  are taken to be the same as the spatial coordinates in the 3 + 1 manifold  $x^i$ .

It is shown in [33] that we can use the inversion Eq. (1.86) and add a factor of  $2\gamma_{k(i}\mathcal{C}_{j)}$  to produce an evolution equation for  $f_{kij}$  that allows the whole evolution system to be symmetric hyperbolic. The resulting system of evolution equations is

$$\partial_t \gamma_{ij} = 2\beta^k f_{kij} + 4\gamma^{lm}(\beta_{(i} f_{j)lm} - f_{lm(i} \beta_{j)}) + 2\gamma_{k(i} \partial_{j)} \beta^k - 2\alpha K_{ij}, \quad (1.93)$$

$$\begin{aligned} \partial_t f_{kij} - \beta^l \partial_l f_{kij} + \alpha \partial_k K_{ij} = & \alpha \{ \gamma^{mn} [4K_{k(i} f_{j)mn} - 4f_{mn(i} K_{j)k} + K_{ij}(2f_{mnk} - 3f_{kmn})] \\ & + 2\gamma^{mn} \gamma^{pq} [K_{mp}(\gamma_{k(i} f_{j)qn} - 2f_{qn(i} \gamma_{j)k}) \\ & + \gamma_{k(i} K_{j)m}(8f_{npq} - 6f_{pqn}) + K_{mn}(4f_{pq(i} \gamma_{j)k} - 5\gamma_{k(i} f_{j)pq})] \\ & - K_{ij} \partial_k \ln \tilde{\alpha} + 2\gamma^{mn} (K_{m(i} \gamma_{j)k} \partial_n \ln \tilde{\alpha} - K_{mn} \gamma_{k(i} \partial_{j)} \ln \tilde{\alpha}) \} \\ & + 2f_{kl(i} \partial_{j)} \beta^l + f_{lij} \partial_k \beta^l + \gamma_{kl} \partial_i \partial_j \beta^l + 16\pi \gamma_{k(i} S_{j)}), \end{aligned} \quad (1.94)$$

$$\begin{aligned} \partial_t K_{ij} - \beta^k \partial_k K_{ij} + \alpha \gamma^{kl} \partial_l f_{kij} = & \alpha \{ \gamma^{kl} (K_{kl} K_{ij} - 2K_{ki} K_{lj}) + \gamma^{kl} \gamma^{mn} (4f_{kmi} f_{[ln]j} \\ & + 4f_{km[n} f_{l]ij} - f_{ikm} f_{jln} + 8f_{(ij)k} f_{[ln]m} + 4f_{km(i} f_{j)ln} \\ & - 8f_{kli} f_{mnj} + 20f_{kl(i} f_{j)mn} - 13f_{ikl} f_{jmn}) - \partial_i \partial_j \ln \tilde{\alpha} \\ & - (\partial_i \ln \tilde{\alpha})(\partial_j \ln \tilde{\alpha}) + 4\gamma_{ij} \gamma^{kl} \gamma^{mn} f_{km[n} \partial_{l]} \ln \tilde{\alpha} \\ & + \gamma^{kl} [(2f_{(ij)k} - f_{kij}) \partial_l \ln \tilde{\alpha} - 3(f_{ikl} \partial_j \ln \tilde{\alpha} + f_{jkl} \partial_i \ln \tilde{\alpha})] \\ & + 4f_{kl(i} \partial_{j)} \ln \tilde{\alpha} \} + 2K_{k(i} \partial_{j)} \beta^k - 8\pi S_{ij} + 4\pi \gamma_{ij} T. \end{aligned} \quad (1.95)$$

This system is complicated, but it has all of the properties that we seek as a starting point for a numerically stable initial boundary value problem. The principal part is written on the left hand side, while source like terms are written on the right hand side. The only reason the source terms in Eq. (1.94) contain the terms in stress-energy tensor is the addition of the term proportional to the Einstein constraints,  $2\gamma_{k(i}\mathcal{C}_{j)}$ . Writing the principal part in matrix form, and performing an eigendecomposition, results in the characteristic modes

$$U_{ij}^+ \equiv -\frac{1}{\sqrt{2}}(K_{ij} + s^k f_{kij}) \sim k^\mu \partial_\mu \gamma_{ij}, \quad (1.96)$$

$$U_{ij}^- \equiv -\frac{1}{\sqrt{2}}(K_{ij} - s^k f_{kij}) \sim \ell^\mu \partial_\mu \gamma_{ij}, \quad (1.97)$$

$$U_{kij}^\perp \equiv \sigma_k^l f_{lij} \sim \sigma_k^\mu \partial_\mu \gamma_{ij}, \quad (1.98)$$

with corresponding characteristic speeds

$$c_\pm = \pm\alpha - s_i \beta^i, \quad c_\perp \equiv -s_i \beta^i. \quad (1.99)$$

The characteristics  $U_{ij}^\pm$  propagate along the light cone, while the characteristics  $U_{kij}^\perp$  propagate along  $n^\mu$ , making all of the propagating degrees of freedom in this system causal.

Analysis of the characteristic matrices shows that this system is symmetric hyperbolic as promised. This ensures that the system has an energy estimate:

$$E_{EC} = \frac{1}{2} \int (\alpha K^{ij} K_{ij} + \alpha f^{kij} f_{kij} - 2K^{ij} \beta^k f_{kij}) dV, \quad (1.100)$$

which is conserved when we consider small high frequency perturbations in the system

$$\partial_t E_{EC} \sim \oint (\alpha K^{ij} - \beta_k f^{kij}) s^l (\alpha f_{lij} - \beta_l K_{ij}) dS. \quad (1.101)$$

Here, a symmetrizer motivated by the energy conservation obeyed by the scalar wave equation on a stationary spacetime is chosen.

The characteristic matrices are only preserved if the gauge is chosen as directed, specifying the densitized lapse and shift for all time. This is because the source terms contain first and second derivatives of  $\tilde{\alpha}$  and  $\beta^i$ , and if these gauge variables were promoted to evolved fields, their derivatives would move into the principal part of the system, directly affecting the characteristic structure. The only way to prevent this would be to specify an evolution scheme third order in derivatives for the gauge variables, and evolve this as a first order system of equations, so that first and second derivatives of the gauge variables become source terms. This comes as a disadvantage for highly dynamical spacetimes, as a user may not know what functions to choose for the gauge variables to ensure the absence of coordinate singularities during the evolution. There do exist elliptic conditions for the lapse and shift that have been shown to prevent coordinate singularities, but these tend to be computationally expensive conditions to implement, and the stability and well-posedness of mixed hyperbolic-elliptic equations can be hard to prove. The advantage of this system however is that there are only 30 evolved fields, whereas the system described in the next section will contain 50 fields, making the Einstein-Christoffel system more efficient with respect to computer memory.

### 1.5.2 The Generalized Harmonic Formulation

The generalized harmonic formulation was first proposed by [34] and was subsequently formalized by [35, 36]. Many successful numerical relativity simulations have since been based on this formulation (for example [38, 39, 40]). The generalized harmonic evolution equations were first written as a symmetric hyperbolic first order system of equations and rigorously numerically tested in [41]. This system will be referred to as a “first order gauge” specification, which is to say that in order to choose the gauge under which the spacetime

will evolve, a user would specify four functions of spacetime that effectively dictate first order evolution equations for the lapse and shift at every point in spacetime. These four functions  $H_\mu$  are defined on a Lorentzian spacetime with metric  $g_{\mu\nu}$  and coordinates  $x^\mu$ :

$$H_\mu(x^\alpha) = -g_{\mu\sigma}\nabla_\nu\nabla^\nu x^\sigma = g^{\alpha\beta}\Gamma_{\mu\alpha\beta} \equiv \Gamma_\mu, \quad (1.102)$$

which can be written as evolution equations for the lapse and shift:

$$\partial_t\alpha - \beta^i\partial_i\alpha = \alpha^2(n^\mu H_\mu - K), \quad (1.103)$$

$$\partial_t\beta^i - \beta^j\partial_j\beta^i = \alpha^2\gamma^{ij}(\gamma^{kl}\Gamma_{jkl} - H_j - \partial_j\ln\alpha). \quad (1.104)$$

The choice  $H_\mu(x^\alpha) = 0$  is called the harmonic coordinate condition. Its usefulness is apparent when we write out the scalar wave equation:

$$\nabla^\mu\nabla_\mu\phi = \partial^\mu\partial_\mu\phi - g^{\mu\nu}\Gamma_{\mu\nu}^\alpha\partial_\alpha\phi = 0 \quad \rightarrow \quad \partial^\mu\partial_\mu\phi = 0. \quad (1.105)$$

This coordinate condition removes first order derivatives of the scalar from the equation, simplifying the corresponding evolution equations. This simplification has been instrumental in various proofs of the well-posedness of Einstein's field equations [42, 43]. By specifying an arbitrary  $H_\mu(x^\alpha)$ , the harmonic simplification may be lost, but the characteristic structure of the scalar field equations is preserved. This is also true of the Einstein field equations, as the specification  $H_\mu(x^\alpha)$  transforms them into a manifestly hyperbolic system. The gauge specification introduces the set of four gauge constraints

$$\mathcal{C}_\mu \equiv \Gamma_\mu - H_\mu, \quad (1.106)$$

which in conjunction with its time derivatives  $\partial_t\mathcal{C}_\mu$ , can be shown to effectively replace the Hamiltonian and momentum constraints introduced in the previous section.

To write the first order evolution equations using this formulation as originally done in [41], we define the variables  $d_{i\mu\nu} \equiv \partial_i g_{\mu\nu}$  to hold information about the spatial derivatives of the metric, and  $P_{\mu\nu} \equiv -n^\alpha\partial_\alpha g_{\mu\nu}$  to hold information about the time derivatives of the metric. The complete state vector for this system can then be written  $\vec{U} = (g_{\mu\nu}, d_{i\mu\nu}, P_{\mu\nu})$ , for a total of 50 evolved fields. The evolution equation for  $g_{\mu\nu}$  comes from the definition of  $P_{\mu\nu}$ , and the evolution of  $P_{\mu\nu}$  comes from the Einstein field equations. Evolution for  $d_{i\mu\nu}$  is achieved by enforcing the commutativity of temporal and spatial derivatives:

$$[\partial_t, \partial_i] = 0, \quad (1.107)$$

and writing

$$\partial_t d_{i\mu\nu} = \partial_k(\beta^i d_{i\mu\nu} - \alpha P_{\mu\nu}). \quad (1.108)$$

The evolution equations are completed by distributing the spatial derivatives and substituting state vector values. The resulting system of evolution equations is

$$\partial_t g_{\mu\nu} = \beta^i d_{i\mu\nu} - \alpha P_{\mu\nu}, \quad (1.109)$$

$$\partial_t d_{i\mu\nu} - \beta^j \partial_j d_{i\mu\nu} + \alpha \partial_i P_{\mu\nu} = \frac{1}{2} \alpha n^\lambda n^\rho d_{i\lambda\rho} P_{\mu\nu} + \alpha \gamma^{jk} n^\lambda d_{ij\lambda} d_{k\mu\nu}, \quad (1.110)$$

$$\begin{aligned} \partial_t P_{\mu\nu} - \beta^i \partial_i P_{\mu\nu} + \alpha \gamma^{ij} \partial_i d_{j\mu\nu} &= 2\alpha g^{\lambda\rho} (\gamma^{ij} d_{i\lambda\mu} d_{j\rho\nu} - P_{\lambda\mu} P_{\rho\nu} - g^{\epsilon\sigma} \Gamma_{\mu\lambda\epsilon} \Gamma_{\nu\rho\sigma}) \\ &\quad + 2\alpha \partial_{(\mu} H_{\nu)} - 2\alpha H_\lambda \Gamma_{\mu\nu}^\lambda - \frac{1}{2} \alpha n^\lambda n^\rho P_{\lambda\rho} P_{\mu\nu} \\ &\quad - \alpha n^\lambda P_{\lambda i} \gamma^{ij} d_{j\mu\nu} - 16\pi \alpha T_{\mu\nu} + 8\pi \alpha g_{\mu\nu} T. \end{aligned} \quad (1.111)$$

where Christoffel symbols are written in terms of the state vector as

$$\Gamma_{\alpha\mu\nu} = n_{(\mu} P_{\nu)\alpha} + d_{i\alpha(\mu} \gamma_{\nu)}^i - \frac{1}{2} (n_\alpha P_{\mu\nu} + \gamma_\alpha^i d_{i\mu\nu}), \quad (1.112)$$

and the lapse and shift are set via the inverse metric components

$$\alpha^2 = (-g^{tt})^{-1}, \quad \beta^i = \alpha^2 g^{ti}. \quad (1.113)$$

This system also has all of the properties that we seek as a starting point for a numerically stable initial boundary value problem. The principal part is identical to the previous system, and the eigendecomposition results in similar characteristic modes

$$U_{\mu\nu}^+ \equiv -\frac{1}{\sqrt{2}} (P_{\mu\nu} + s^\alpha d_{\alpha\mu\nu}) = k^\alpha \partial_\alpha g_{\mu\nu}, \quad (1.114)$$

$$U_{\mu\nu}^- \equiv -\frac{1}{\sqrt{2}} (P_{\mu\nu} - s^\alpha d_{\alpha\mu\nu}) = \ell^\alpha \partial_\alpha g_{\mu\nu}, \quad (1.115)$$

$$U_{\alpha\mu\nu}^\perp \equiv \sigma_\alpha^\beta d_{\beta\mu\nu} = \sigma_\alpha^\mu \partial_\mu g_{\mu\nu}, \quad (1.116)$$

with corresponding characteristic speeds

$$c_\pm = \pm \alpha - s_i \beta^i, \quad c_\perp \equiv -s_i \beta^i. \quad (1.117)$$

The characteristics  $U_{\mu\nu}^\pm$  propagate along the light cone, while the characteristics  $U_{\alpha\mu\nu}^\perp$  propagate along  $n^\mu$ , making all of the propagating degrees of freedom in this system causal.

The energy estimate for this system can be written as

$$E_{GH} = \frac{1}{2} \int m^{\mu\nu} m^{\epsilon\sigma} \left[ \alpha (P_{\mu\epsilon} P_{\nu\sigma} + d_{\mu\epsilon}^i d_{i\nu\sigma}) - 2\beta^i P_{\mu\epsilon} d_{i\nu\sigma} \right] dV, \quad (1.118)$$

where  $m^{\mu\nu}$  is any positive definite metric. Here, a symmetrizer motivated by the energy conservation obeyed by the scalar wave equation on a stationary spacetime is chosen. This

energy estimate is conserved when we consider small high frequency perturbations in the system:

$$\partial_t E_{GH} \sim \oint m^{\mu\nu} m^{\epsilon\sigma} (\alpha P_{\mu\epsilon} - \beta^j d_{j\mu\epsilon}) s_i (\alpha d^i_{\nu\sigma} - \beta^i P_{\nu\sigma}) dS. \quad (1.119)$$

It will be demonstrated in Chapter 3 that instead of distributing the spatial derivatives as was done in the system above, the principal part can be written in a form more akin to the flux conservative form common in hydrodynamic systems to better adhere to summation by parts energy estimates. The system shown here is more directly representative of that originally given by [41] to draw a direct comparison to the principal parts of the Einstein-Christoffel system and the generalized harmonic system.

## Chapter 2

# Numerical Relativity in Spherical Symmetry

### Preface

This chapter contains the work published in [\[44\]](#) titled “Reflecting boundary conditions in numerical relativity as a model for black hole echoes”. It has not been altered from its published version other than to adjust some equations to better adhere to the formatting of this thesis. References to ‘we’ in this chapter either refer to the list of authors in [\[44\]](#) (Conner Dailey, Niayesh Afshordi, and Erik Schnetter), or to these authors and the reader.

This work represents the usual first step in numerical relativity whenever a new concept, numerical technique, or formulation is introduced, which is to implement it first within the simplification of spherical symmetry. This makes the problem effectively one dimensional, which is simple to implement, computationally inexpensive, and acts as a stage to correct common mistakes and to make headway in understanding.

In this case, it acts as a stage in which to experiment with reflecting boundary conditions within numerical relativity.

## 2.1 Introduction

The recent discovery of gravitational waves (GWs) has led to the new field of GW astronomy, opening novel windows into some of the deepest physical mysteries in our universe. Chief amongst these is the true nature of black hole horizons, which appear to have both temperature and entropy, if one applies laws of quantum mechanics to the fields in their vicinity [45, 46]. Yet, according to Einstein’s theory of General Relativity (GR), horizons comprise nothing but empty space. Even more problematic is when the thermal nature of black holes (i.e. Hawking radiation) leads to their evaporation, leaving us to wonder what happens to the information behind the horizon that cannot escape due to relativistic causality. This is known as the black hole information paradox [47, 48]. Given that GW astronomy can now probe into the vicinity of black hole horizons, it is natural to ask whether it can give us an empirical window into resolving these theoretical mysteries. In particular, one may wonder whether quantum effects near the horizon would lead to echoes in observations that would have been absent in GR with classical horizons [49].

Motivated by this, there has been a recent interest in modelling black hole echoes phenomenologically [50, 13, 51, 16, 52, 53, 49, 15, 54]. The idea behind black hole echoes is that there may be some mechanism, resulting from quantum phenomena for example, by which wave packets falling into a black hole could partially reflect off of an interface before reaching the horizon, thus resulting in a potentially detectable effect. In the context of GW astronomy, this has opened a novel window to study exotic near-horizon physics phenomenologically, from current and future observations [52, 53, 49, 54]. However, interpreting this data requires modelling strong gravitational systems in numerical relativity, where there does not currently seem to be a good understanding of how to properly implement a reflecting surface (but see [55] for an approximate method and [56] for an adjacent approach to boundaries). There has also been some recent skepticism that black hole echoes can be detected at all due to the formation of an apparent horizon before the reflection occurs [57], and having a proper way to model reflecting surfaces allows for rigorous testing beyond order-of-magnitude estimates.

One way to implement a reflecting surface is to have an artificial boundary in the domain of the numerical problem where the surface is to be located, and impose a set of boundary conditions (BCs) there. This requires an understanding of the full initial boundary value problem (IBVP) for a particular framework of numerical relativity, which the majority of studies tend to avoid by imposing no boundaries or by having boundaries out of causal contact with the initial conditions. This work contains some examples of the full spherically symmetric IBVP in numerical relativity with a scalar field. Of course there are no GWs in spherical symmetry, but see Appendix A for how this can be done

analogously in cylindrical symmetry.

The generic way of treating the BCs in hyperbolic systems of partial differential equations is to identify the characteristic modes and speeds of the system, and for each mode that has a characteristic speed leading it out of the domain, no BCs are applied, while all of the modes propagating into the domain require a boundary treatment. It is then advantageous to pick a formulation of Einstein's equations where the characteristic modes and speeds are simple and well-behaved. Here, the Einstein-Christoffel (EC) formulation is used due to its simple characteristic structure, symmetric hyperbolicity, and previously successful numerical implementation [37].

In Section 2.2, we describe the EC system and the scalar field equations adapted from [37]. In Section 2.3, we derive BCs based on conservation laws while Section 2.4 dictates the initial conditions we consider. Section 2.5 describes our numerical implementation using summation by parts (SBP) operators and BCs implemented with simultaneous approximation terms (SATs). Finally, we present our results for several reflecting IBVPs in Section 2.6, discuss near-horizon boundaries, and discuss the evolution of the apparent horizon as a response to [57].

## 2.2 Theoretical Framework for the Einstein-Christoffel system

In general, the physical metric  $g_{\mu\nu}$  in spherical symmetry can be expressed with respect to the spherical coordinates  $x^\alpha = (t, r, \theta, \varphi)$ , with the line element:

$$ds^2 = -\alpha^2 dt^2 + \gamma_{rr}(dr + \beta^r dt)^2 + \gamma_{\theta\theta} d\Omega^2, \quad (2.1)$$

where  $\alpha$  is the lapse,  $\beta^r$  is the shift, and  $\gamma_{ij}$  are elements of the 3-metric. The extrinsic curvature is defined as

$$K_{ij} = -\frac{1}{2\alpha} (\partial_t - \mathcal{L}_\beta) \gamma_{ij}, \quad (2.2)$$

where  $\mathcal{L}_\beta$  represents the Lie derivative with respect to the shift vector. In order to make the evolution equations first order in space, the functions

$$f_{kij} \equiv \Gamma_{(ij)k} + \gamma_{ki} \gamma^{lm} \Gamma_{[lj]m} + \gamma_{kj} \gamma^{lm} \Gamma_{[li]m}, \quad (2.3)$$

are defined. Here,  $\Gamma^k_{ij}$  are the Christoffel symbols associated with the 3-metric. The EC framework leaves the densitized lapse  $\tilde{\alpha} \equiv \alpha/(\sqrt{\gamma_{rr}\gamma_{\theta\theta}})$  and the shift as freely specifiable

gauge functions. It is understood that wherever  $\alpha$  may appear in the evolution equations, it is set with  $\alpha = \tilde{\alpha}\sqrt{\gamma_{rr}}\gamma_{\theta\theta}$ . While we present a general formalism in what follows, we shall come back to our particular choice of gauge in Section (2.2.3).

### 2.2.1 The Einstein-Christoffel vacuum equations

The evolution equations in the EC system in spherical symmetry were introduced in detail in [37], which we modify to the following form:

$$\partial_t \gamma_{rr} - \beta^r \partial_r \gamma_{rr} = 2\gamma_{rr} \partial_r \beta^r - 2\alpha K_{rr}, \quad (2.4)$$

$$\partial_t \gamma_{\theta\theta} - \beta^r \partial_r \gamma_{\theta\theta} = -2\alpha K_{\theta\theta}, \quad (2.5)$$

$$\begin{aligned} \partial_t K_{rr} - \beta^r \partial_r K_{rr} + \alpha \mathcal{D}^r f_{rrr} = & 3 \frac{\alpha f_{rrr}^2}{\gamma_{rr}^2} - 6 \frac{\alpha f_{r\theta\theta}^2}{\gamma_{\theta\theta}^2} - \frac{\alpha K_{rr}^2}{\gamma_{rr}} + 2 \frac{\alpha K_{rr} K_{\theta\theta}}{\gamma_{\theta\theta}} - 10 \frac{\alpha f_{rrr} f_{r\theta\theta}}{\gamma_{rr} \gamma_{\theta\theta}} \\ & - \frac{\alpha f_{rrr} \partial_r \ln \tilde{\alpha}}{\gamma_{rr}} - \alpha (\partial_r \ln \tilde{\alpha})^2 - \alpha \partial_r^2 \ln \tilde{\alpha} + 2K_{rr} \partial_r \beta^r, \end{aligned} \quad (2.6)$$

$$\partial_t K_{\theta\theta} - \beta^r \partial_r K_{\theta\theta} + \alpha \mathcal{D}^r f_{r\theta\theta} = \alpha + \frac{\alpha K_{rr} K_{\theta\theta}}{\gamma_{rr}} + \frac{\alpha f_{rrr} f_{r\theta\theta}}{\gamma_{rr}^2} - 4 \frac{\alpha f_{r\theta\theta}^2}{\gamma_{rr} \gamma_{\theta\theta}} - \frac{\alpha f_{r\theta\theta} \partial_r \ln \tilde{\alpha}}{\gamma_{rr}}, \quad (2.7)$$

$$\begin{aligned} \partial_t f_{rrr} - \beta^r \partial_r f_{rrr} + \alpha \partial_r K_{rr} = & 12 \frac{\alpha \gamma_{rr} K_{\theta\theta} f_{r\theta\theta}}{\gamma_{\theta\theta}^2} - \frac{\alpha K_{rr} f_{rrr}}{\gamma_{rr}} - 10 \frac{\alpha K_{rr} f_{r\theta\theta}}{\gamma_{\theta\theta}} - 4 \frac{\alpha K_{\theta\theta} f_{rrr}}{\gamma_{\theta\theta}} \\ & - \alpha K_{rr} \partial_r \ln \tilde{\alpha} - 4 \frac{\alpha \gamma_{rr} K_{\theta\theta} \partial_r \ln \tilde{\alpha}}{\gamma_{\theta\theta}} + 3 f_{rrr} \partial_r \beta^r + \gamma_{rr} \partial_r^2 \beta^r, \end{aligned} \quad (2.8)$$

$$\partial_t f_{r\theta\theta} - \beta^r \partial_r f_{r\theta\theta} + \alpha \partial_r K_{\theta\theta} = 2 \frac{\alpha K_{\theta\theta} f_{r\theta\theta}}{\gamma_{\theta\theta}} - \frac{\alpha K_{\theta\theta} f_{rrr}}{\gamma_{rr}} - \alpha K_{\theta\theta} \partial_r \ln \tilde{\alpha} + f_{r\theta\theta} \partial_r \beta^r. \quad (2.9)$$

There are a few differences in this form of the equations compared to those presented in [37]. First, we write the equations explicitly in terms of the operator  $\mathcal{D}^i$ , which acts on a 3-covector  $f_i$  as  $\mathcal{D}^i f_i = (\sqrt{\gamma})^{-1} \partial^i (\sqrt{\gamma} f_i)$  (reasons for this will be given in Section 2.5.1). Also, instead of defining transverse elements like  $\gamma_T = \gamma_{\theta\theta}/r^2$ , we keep the evolution equations in a form that does not explicitly depend on the coordinates. The principal part of this system makes up the left hand side and source-like terms make up the right hand side, which suggests the simple characteristic structure of this formulation of Einstein's vacuum equations. We should note that there is only gauge dynamics possible in the above system until we add stress-energy terms, which we do next.

### 2.2.2 Scalar Field and Source Terms

Scalar fields of mass  $m$  are subject to the Klein-Gordon equation  $\nabla^\mu \nabla_\mu \phi - m^2 \phi = 0$ . This equation can be reduced to a first order system and keep the same characteristic structure as the EC system with the definition of two auxiliary variables:  $\psi_r \equiv \partial_r \phi$  and  $\Pi \equiv -(\partial_t \phi - \beta^r \partial_r \phi)/\alpha$ . The evolution equations then become

$$\partial_t \phi - \beta^r \partial_r \phi = -\alpha \Pi, \quad (2.10)$$

$$\partial_t \psi_r - \beta^r \partial_r \psi_r + \alpha \partial_r \Pi = \alpha \left( -\frac{f_{rrr}}{\gamma_{rr}} + 2\frac{f_{r\theta\theta}}{\gamma_{\theta\theta}} - \partial_r \ln \tilde{\alpha} \right) \Pi + \partial_r \beta^r \psi_r, \quad (2.11)$$

$$\partial_t \Pi - \beta^r \partial_r \Pi + \alpha \mathcal{D}^r \psi_r = \alpha \left( \frac{K_{rr}}{\gamma_{rr}} + 2\frac{K_{\theta\theta}}{\gamma_{\theta\theta}} \right) \Pi + \frac{\alpha}{\gamma_{rr}} \left( \frac{f_{rrr}}{\gamma_{rr}} - 6\frac{f_{r\theta\theta}}{\gamma_{\theta\theta}} - \partial_r \ln \tilde{\alpha} \right) \psi_r + m^2 \alpha \phi. \quad (2.12)$$

With the unit normal to the spatial foliation  $n_\mu$ , the stress-energy tensor  $T^{\mu\nu}$  is decomposed into the energy density  $\rho = n_\mu n_\nu T^{\mu\nu}$ , the momentum density  $S_i = -\gamma_{i\mu} n_\nu T^{\mu\nu}$ , the trace  $T = T^\mu_\mu$ , and the spatial stress  $S_{ij} = \gamma_{i\mu} \gamma_{j\nu} T^{\mu\nu}$ . In spherical symmetry the nonzero elements for the Klein-Gordon field are explicitly

$$\rho = (\Pi^2 + \psi_r \psi^r + m^2 \phi^2) / 2, \quad (2.13)$$

$$S_r = \Pi \psi_r, \quad (2.14)$$

$$T = \Pi^2 - \psi_r \psi^r - 2m^2 \phi^2, \quad (2.15)$$

$$S_{rr} = \gamma_{rr} (\Pi^2 + \psi_r \psi^r - m^2 \phi^2) / 2, \quad (2.16)$$

$$S_{\theta\theta} = \gamma_{\theta\theta} (\Pi^2 - \psi_r \psi^r - m^2 \phi^2) / 2. \quad (2.17)$$

These elements modify the right hand side Eqns. (2.6-2.8) in this framework as

$$\partial_t K_{rr} = \dots + 4\pi\alpha(\gamma_{rr}T - 2S_{rr}), \quad (2.18)$$

$$\partial_t K_{\theta\theta} = \dots + 4\pi\alpha(\gamma_{\theta\theta}T - 2S_{\theta\theta}), \quad (2.19)$$

$$\partial_t f_{rrr} = \dots + 16\pi\alpha\gamma_{rr}S_r, \quad (2.20)$$

and this system is subject to a set of five constraints:

$$C \equiv \frac{\partial_r f_{r\theta\theta}}{\gamma_{rr}\gamma_{\theta\theta}} + \frac{7}{2} \frac{f_{r\theta\theta}^2}{\gamma_{rr}\gamma_{\theta\theta}^2} - \frac{f_{rrr}f_{r\theta\theta}}{\gamma_{rr}^2\gamma_{\theta\theta}} - \frac{1}{2} \frac{K_{\theta\theta}^2}{\gamma_{\theta\theta}^2} - \frac{1}{2\gamma_{\theta\theta}} - \frac{K_{rr}K_{\theta\theta}}{\gamma_{rr}\gamma_{\theta\theta}} + 4\pi\rho = 0, \quad (2.21)$$

$$C_r \equiv \frac{\partial_r K_{\theta\theta}}{\gamma_{\theta\theta}} - \frac{K_{\theta\theta}f_{r\theta\theta}}{\gamma_{\theta\theta}^2} - \frac{K_{rr}f_{r\theta\theta}}{\gamma_{rr}\gamma_{\theta\theta}} + 4\pi S_r = 0, \quad (2.22)$$

$$C_{rrr} \equiv \partial_r \gamma_{rr} + 8 \frac{\gamma_{rr}f_{r\theta\theta}}{\gamma_{\theta\theta}} - 2f_{rrr} = 0, \quad (2.23)$$

$$C_{r\theta\theta} \equiv \partial_r \gamma_{\theta\theta} - 2f_{r\theta\theta} = 0, \quad (2.24)$$

$$C_\phi \equiv \partial_r \phi - \psi_r = 0. \quad (2.25)$$

Eqns. (2.21) and (2.22) are the Hamiltonian and Momentum constraints respectively, Eqns. (2.23) and (2.24) come from definition Eq. (2.3), and Eq. (2.25) was defined at the beginning of this section.

The characteristic modes for the complete system of equations include a set of three modes that propagate along the timelike normal to the foliation with characteristic speed  $-\beta^r$ :

$$U_r^0 = \gamma_{rr}, \quad U_\theta^0 = \gamma_{\theta\theta}, \quad U_\phi^0 = \phi, \quad (2.26)$$

and a set of six modes that propagate along the light cone with characteristic speeds  $c_\pm \equiv -\beta^r \pm \alpha/\sqrt{\gamma_{rr}}$ :

$$U_r^\pm = K_{rr} \pm \frac{f_{rrr}}{\sqrt{\gamma_{rr}}}, \quad (2.27)$$

$$U_\theta^\pm = K_{\theta\theta} \pm \frac{f_{r\theta\theta}}{\sqrt{\gamma_{rr}}}, \quad (2.28)$$

$$U_\phi^\pm = \Pi \pm \frac{\psi_r}{\sqrt{\gamma_{rr}}}. \quad (2.29)$$

### 2.2.3 Gauge Choices in the Bulk

In this work, we will consider one particular gauge choice, that is that  $\tilde{\alpha}$  and  $\beta^r$  are time independent:

$$\partial_t \tilde{\alpha} = \partial_t \beta^r = 0. \quad (2.30)$$

Other types of gauge choices have been discussed in [37], but it is not clear to us that many of these choices do not change the characteristic structure of the evolution equations. If one considers a hyperbolic time evolution of the gauge variables, in general this will directly affect the characteristic structure, but it is not clear whether the characteristics are well-defined if  $\tilde{\alpha}$  and  $\beta^r$  are prescribed with elliptic gauge conditions. Therefore, we restrict our analysis to our gauge choice Eq. (2.30), where it is clear that the characteristic structure is as presented in the previous section, and leave other gauge choices for future work.

## 2.3 Boundary Conditions

We now restrict the problem to a spatial domain where  $r \in [a, b]$ . One way to gain some intuition on BCs for the scalar wave equation is to study the case of a static background. In such a case we have a time-like Killing vector  $\xi^\nu$  and thus a conserved current  $J^\mu = \xi^\nu T^\mu_\nu$ . We then define the static energy

$$E_s = \int_a^b (\alpha\rho - \beta^r S_r) \sqrt{\gamma} dr, \quad (2.31)$$

and rewrite the conservation law  $\nabla_\mu J^\mu = 0$  in terms of the characteristics

$$\partial_t E_s = \frac{1}{4} \sqrt{\gamma_{rr}} \sqrt{\gamma} [(c_- U_\phi^-)^2 - (c_+ U_\phi^+)^2] \Big|_a^b. \quad (2.32)$$

The flux term on the right hand side suggests the BCs that can be applied to allow  $E_s$  to enter/leave the domain:

$$U_\phi^+ = -k_a \frac{c_-}{c_+} U_\phi^- \quad \text{at } r = a, \quad (2.33)$$

$$U_\phi^- = -k_b \frac{c_+}{c_-} U_\phi^+ \quad \text{at } r = b, \quad (2.34)$$

for some coefficients  $k_{a,b}$ . While  $k_{a,b}$  do not necessarily need to be constants, the values  $k_{a,b} = \pm 1$  keep  $E_s$  exactly conserved in the domain for each boundary. In this work, a conservative BC that reverses the sign of an incoming pulse is referred to as a Dirichlet type ( $k_{a,b} = -1$ ), while one that retains the sign is referred to as a Neumann type ( $k_{a,b} = +1$ ). The motivation for this naming scheme comes from the fact that these BCs reduce to the classical Dirichlet ( $\partial_t \phi = 0$ ) and Neumann ( $\partial_r \phi = 0$ ) BCs in Minkowski space where  $c_\pm = \pm 1$ . It is important to note that we are considering domains and gauge conditions where  $c_+ c_- < 0$  throughout so that both boundaries always require BCs.

Once the metric becomes time dependent,  $J^\mu$  is no longer conserved. Instead, the notion of what a reflection means needs to be rooted in a quantity that describes energy in a dynamical spacetime. One way of defining this is with the Misner-Sharp mass, which in spherical symmetry can be written as [37]

$$M(r) = \frac{\sqrt{\gamma_{\theta\theta}}}{2} \left( 1 + \frac{U_\theta^+ U_\theta^-}{\gamma_{\theta\theta}} \right). \quad (2.35)$$

To obtain the BCs on the incoming scalar modes  $U_\phi^\pm$ , we express the derivatives of the Misner-Sharp mass in terms of the state vector:

$$\begin{aligned} \partial_t M &= 4\pi\sqrt{\gamma_{\theta\theta}} [f_{r\theta\theta}(\beta^r \rho - \alpha S_r / \gamma_{rr}) \\ &\quad + K_{\theta\theta}(\alpha \rho + \alpha T - 2\alpha S_{\theta\theta} / \gamma_{\theta\theta} - \beta^r S_r)] , \end{aligned} \quad (2.36)$$

$$\partial_r M = 4\pi\sqrt{\gamma_{\theta\theta}}(f_{r\theta\theta}\rho - K_{\theta\theta}S_r). \quad (2.37)$$

These relationships can be derived by taking the appropriate derivative of Eq. (2.35) and substituting time derivatives with the evolution equations and spatial derivatives with the constraints. It is interesting that these relationships can be expressed solely in terms of the state vector, which enables us to impose BCs on the scalar characteristics to control  $M$ .

To see this, let us integrate Eq. (2.37) to define the Misner-Sharp “energy” enclosed within our domain

$$E_M = \int_a^b \frac{f_{r\theta\theta}\rho - K_{\theta\theta}S_r}{\sqrt{\gamma_{rr}\gamma_{\theta\theta}}} \sqrt{\gamma} dr. \quad (2.38)$$

In the continuum, we clearly have  $E_M = M(b) - M(a)$ . We can then write a conservation law by taking a time derivative and substituting Eq. (2.36). Written here for a massless scalar (i.e.,  $m = 0$ ), we have

$$\partial_t E_M = \frac{\sqrt{\gamma}}{4\sqrt{\gamma_{\theta\theta}}} [c_+ U_\theta^- (U_\phi^+)^2 - c_- U_\theta^+ (U_\phi^-)^2] \Big|_a^b. \quad (2.39)$$

The flux term on the right hand side suggests the general BCs that can be applied to allow  $E_M$  to enter/leave the domain:

$$U_\phi^+ = k_a \sqrt{\frac{c_- U_\theta^+}{c_+ U_\theta^-}} U_\phi^- \quad \text{at } r = a, \quad (2.40)$$

$$U_\phi^- = k_b \sqrt{\frac{c_+ U_\theta^-}{c_- U_\theta^+}} U_\phi^+ \quad \text{at } r = b, \quad (2.41)$$

where the coefficient values  $k_{a,b} = \mp 1$  define the Dirichlet/Neumann type BCs on the scalar characteristics that keep  $E_M$  exactly conserved at each boundary. Interestingly, in the case of  $\partial_t \gamma_{\theta\theta} = 0$ , these reduce to the static background BCs, Eqns. (2.33-2.34), which motivates their connection to the classical Dirichlet/Neumann BCs.

The expansion of outgoing null geodesics is proportional to the value of  $U_\theta^-$ , and thus the apparent horizon is the outermost surface where  $U_\theta^- = 0$ . We call the surface where  $c_+ = 0$  the characteristic horizon. Only when  $c_+ < 0$  are BCs no longer required at  $r = a$  as both characteristics are then leaving the domain. If  $c_+ c_- < 0$  and  $-U_\theta^- U_\theta^+ < 0$ , i.e. the boundary  $r = a$  is between the apparent horizon and the characteristic horizon, the BCs at  $r = a$  are not well-defined unless  $k_a = 0$ . We will not consider any simulations where such cases are present in this work.

The BCs on the incoming angular characteristics  $U_\theta^\pm$  are given by Eq. (2.35):

$$U_\theta^+ = \frac{2M(a)\sqrt{\gamma_{\theta\theta}} - \gamma_{\theta\theta}}{U_\theta^-} \quad \text{at } r = a, \quad (2.42)$$

$$U_\theta^- = \frac{2M(b)\sqrt{\gamma_{\theta\theta}} - \gamma_{\theta\theta}}{U_\theta^+} \quad \text{at } r = b, \quad (2.43)$$

where the values of  $M(a)$  and  $M(b)$  at each time step are given by integrating their time derivatives with the scalar BCs applied

$$\partial_t M(a) = -\pi \tau_a c_- \sqrt{\gamma_{rr} \gamma_{\theta\theta}} U_\theta^+ (U_\phi^-)^2 \quad \text{at } r = a, \quad (2.44)$$

$$\partial_t M(b) = \pi \tau_b c_+ \sqrt{\gamma_{rr} \gamma_{\theta\theta}} U_\theta^- (U_\phi^+)^2 \quad \text{at } r = b, \quad (2.45)$$

where  $\tau_{a,b} = (1 - k_{a,b}^2)$ . We thus see that, in the case of Dirichlet/Neumann type BCs, the Misner-Sharp mass at both boundaries remains constant.

As long as  $\beta^r > 0$ , the boundary  $r = b$  has three additional incoming modes  $U_r^0$ ,  $U_\theta^0$ , and  $U_\phi^0$ . As suggested in [58], these can all be fixed using the constraints (2.23-2.25) by replacing the  $r$  derivatives in their evolution equations:

$$\partial_t \phi = \beta^r (\psi_r) - \alpha \Pi, \quad (2.46)$$

$$\begin{aligned} \partial_t \gamma_{rr} = \beta^r \left( 2f_{rrr} - 8 \frac{\gamma_{rr} f_{r\theta\theta}}{\gamma_{\theta\theta}} \right) \\ + 2\gamma_{rr} \partial_r \beta^r - 2\alpha K_{rr}, \end{aligned} \quad (2.47)$$

$$\partial_t \gamma_{\theta\theta} = \beta^r (2f_{r\theta\theta}) - 2\alpha K_{\theta\theta}, \quad (2.48)$$

all evaluated at  $r = b$ .

While fixing the masses  $M(a)$  and  $M(b)$ , and scalar characteristics (Eqs. 2.40-2.41), fixes all the physical degrees of freedom at the boundaries, the incoming radial characteristics  $U_r^\pm$  are left arbitrary, and thus should be connected to the residual gauge freedoms. Although we have specified the gauge dynamics in the bulk by choosing  $\tilde{\alpha}$  and  $\beta^r$ , additional gauge freedom can propagate into the domain from outside, and thus needs to be specified by fixing the incoming radial modes.

We shall consider a few choices for the BCs of  $U_r^\pm$ . First, one could impose  $\partial_t U_r^\pm = 0$  at the corresponding boundaries:

$$U_r^+(t) = U_r^+(0) \quad \text{at } r = a, \quad (2.49)$$

$$U_r^-(t) = U_r^-(0) \quad \text{at } r = b, \quad (2.50)$$

which ensures there are no incoming radial characteristics into the domain. Next, we could impose  $\partial_t K_{rr} = 0$ :

$$U_r^+(t) = -U_r^-(t) + 2K_{rr}(0) \quad \text{at } r = a, \quad (2.51)$$

$$U_r^-(t) = -U_r^+(t) + 2K_{rr}(0) \quad \text{at } r = b, \quad (2.52)$$

and finally we could impose  $\partial_t f_{rrr} = 0$ :

$$U_r^+(t) = U_r^-(t) - \frac{2f_{rrr}(0)}{\sqrt{\gamma_{rr}(t)}} \quad \text{at } r = a, \quad (2.53)$$

$$U_r^-(t) = U_r^+(t) + \frac{2f_{rrr}(0)}{\sqrt{\gamma_{rr}(t)}} \quad \text{at } r = b, \quad (2.54)$$

It is not clear if different choices may be more advantageous, but we find that for long term stability, the condition  $\partial_t K_{rr} = 0$  at both boundaries seems to work the best.

## 2.4 Initial Conditions

For the initial background, we consider a Schwarzschild black hole in Kerr-Schild coordinates, but with a  $r$ -dependent mass function:

$$\alpha^{-2} = 1 + \frac{2M(r,0)}{r}, \quad \beta^r = \frac{2M(r,0)}{r}\alpha^2, \quad \gamma_{rr} = \alpha^{-2}, \quad \gamma_{\theta\theta} = r^2, \quad (2.55)$$

The initial values of  $f_{rrr}$  and  $f_{r\theta\theta}$  are formed from constraint Eqs. (2.23) and (2.24). The initial values of extrinsic curvature components are formed via Eqs. (2.4) and (2.5), with

$\partial_t \gamma_{\theta\theta} = 0$  assumed, but  $\partial_t \gamma_{rr}$  kept arbitrary. The yet unspecified functions  $M(r, 0)$  and  $\partial_t \gamma_{rr}$  will be used to satisfy the constraints. For the scalar field, a spherical pulse of amplitude  $A$ , total width  $2\sigma$ , and location  $\mu$  is modeled as a section of a polynomial:

$$\phi(r, 0) = \frac{A}{r\sigma^8} [r - (\mu - \sigma)]^4 [r - (\mu + \sigma)]^4, \quad (2.56)$$

and is set to zero outside of  $(\mu - \sigma) \leq r \leq (\mu + \sigma)$ . The degree of this polynomial assures that the first three derivatives are continuous. The initial condition on  $\psi_r$  is obtained by taking the  $r$  derivative. For the initial condition on  $\Pi$ , a common choice is  $\Pi = 0$ , which describes a pulse that will break into two parts traveling at speeds  $c_+$  and  $c_-$ . Another choice is to specify that the pulse is initially traveling at speed  $c_-$ , such that the initial time derivative is

$$\partial_t \phi(r, 0) = -\frac{8Ac_-}{r\sigma^8} [(r - \mu)^2 - \sigma^2]^3 (r - \mu), \quad (2.57)$$

and is zero outside of  $(\mu - \sigma) \leq r \leq (\mu + \sigma)$ . The initial value of  $\Pi$  is then completed with the definition  $\Pi = -(\partial_t \phi - \beta^r \psi_r)/\alpha$ . Given initial conditions on the scalar field, the Hamiltonian and momentum constraints must be satisfied at the initial time. With the two functions  $M(r, 0)$  and  $\partial_t \gamma_{rr}$ , one can show that these constraints are satisfied if

$$\partial_r M(r, 0) = 4\pi r^2 (\alpha \rho - \beta^r S_r) / \alpha, \quad (2.58)$$

$$\partial_t \gamma_{rr} = -8\pi r S_r / \alpha. \quad (2.59)$$

These are easy conditions to satisfy, as  $M(r, 0)$  can be integrated with a standard solver starting at  $r = a$  with initial internal mass  $M_0$  or from  $r = b$  with initial total mass  $M_{\text{tot}}$ . The value of  $\partial_t \gamma_{rr}$  can be replaced outright in the initial value of  $K_{rr}$ .

## 2.5 Numerical Implementation

In this section, we will introduce our numerical implementation of the IBVPs we are considering. We use Summation-By-Parts (SBP) derivative operators in an effort to preserve numerical stability by ensuring the energy of the system is bounded. In order to impose boundary conditions (BCs) in a stable fashion we use simultaneous approximation terms (SATs). Finally, we use numerical dissipation to prevent instability due to high-frequency noise.

### 2.5.1 Summation-By-Parts Derivative Operators

A popular way to maintain stability in numerical hyperbolic IBVPs is to use finite differencing operators that satisfy SBP, which is the discrete analog of integration by parts. Using SBP operators can be proven to be closely related to the well-posedness and the numerical stability of many conservative problems [29, 30]. In order to introduce our covariant SBP scheme, we review some covariant integration properties. In a 3-dimensional domain  $V$  with coordinates  $x$  and the 2-dimensional boundary of that domain  $\partial V$  with coordinates  $\xi$ , the covariant Gauss's theorem states that for a vector field  $F^i$

$$\int_V \nabla_i F^i \sqrt{\gamma} d^3x = \oint_{\partial V} n_i F^i \sqrt{s} d^2\xi, \quad (2.60)$$

where the determinants of the metric on  $V$  and  $\partial V$  are  $\gamma$  and  $s$  respectively and  $n_i$  is the unit normal to the boundary  $\partial V$ . If the vector field is represented by a scalar factor and a vector factor as  $F^i = uv^i$ , in spherical symmetry, this property can be written as

$$\int_a^b u \nabla_r v^r \sqrt{\gamma} dr + \int_a^b (\partial_r u) v^r \sqrt{\gamma} dr = uv^r \sqrt{\gamma} \Big|_a^b, \quad (2.61)$$

where  $\nabla_r v^r = (\sqrt{\gamma})^{-1} \partial_r (\sqrt{\gamma} v^r)$  is the covariant divergence. This can be thought of as the covariant version of integration by parts in 1-dimension. Our goal will be to develop a numerical implementation of our IBVP that obeys a discrete analog of this property in an effort to maintain numerical stability.

For our spatial domain  $r \in [a, b]$  we define a grid where all functions will be sampled with  $n$  points spaced by a distance  $h$ . An  $n \times n$  finite differencing operator  $D$  paired with a symmetric and positive definite  $n \times n$  norm operator  $\Sigma$  are said to satisfy SBP if [29]

$$\Sigma D + D^T \Sigma = B, \quad (2.62)$$

where the boundary operator  $B = \text{diag}(-1, 0, \dots, 0, 1)$ . For this property to mimic the covariant property Eq. (2.61), we insert a matrix  $\Gamma$  with the values of  $\sqrt{\gamma}$  injected along the diagonal:

$$W \nabla + D^T W = B \Gamma. \quad (2.63)$$

The operator  $\nabla \equiv \Gamma^{-1} D \Gamma$  approximates the covariant 3-divergence of 3-vectors, the operator  $D$  approximates the covariant scalar gradient, and  $W \equiv \Sigma \Gamma$  is the covariant norm

operator and approximates covariant integration. Then, in one spatial dimension, for a scalar grid function  $u$  and the one non-zero component of a 3-vector grid function  $v^r$ ,

$$u^T W \nabla v^r + (Du)^T W v^r = uv^r \sqrt{\gamma} \Big|_a^b, \quad (2.64)$$

which directly mimics the continuous property Eq. (2.61).

In the case of the wave equation on a static background, one can write the energy conservation law in a directly analogous way to the covariant property Eq. (2.61) (see Appendix B), and thus when the system is discretized using the SBP operators, the system remains strictly stable in the sense that the energy is bounded [29, 30]. It is no longer clear how to properly do this when the spacetime becomes dynamic. The state vector in the EC system is defined in terms of lower-index functions ( $f_{ijk}$ ), which runs counter to the covariant SBP property that is defined in terms of an upper-index function. We have discovered one way that seems to be stable in at least all of the cases considered here, but a more elegant discretization paradigm may exist, perhaps one where the SBP properties can be made to mimic the dynamic conservation law Eq. (2.39), and the equations of motion can be written in terms of covariant divergences of upper-index functions. In the numerical scheme presented here, the evolution equations written in Section 2.2 are discretized by replacing scalar gradients with an SBP operator (i.e.  $\partial_r \rightarrow D$ ) and where present the operator  $\mathcal{D}_r \rightarrow \Gamma^{-1} D \Gamma$ .

In this work, we use the  $D_{6-3}$  SBP operator defined in [59] that minimizes the so-called average boundary truncation error. This operator is 6<sup>th</sup> order accurate in the interior and 3<sup>rd</sup> order accurate near the boundaries. It was reported in [59] that this operator achieves near 4<sup>th</sup> order global convergence with a diagonal norm operator, which in principle will pair nicely with standard 4<sup>th</sup> order Runge-Kutta time integration.

### 2.5.2 Application of Boundary Conditions

The BCs are applied using SATs. This method applies BCs in a weak fashion, adding an exponential decay term to the evolution equations at the boundary. For two arbitrary characteristic grid functions  $U^\pm(r, t)$  with characteristic speeds  $c_\pm$ , the application of the general BCs  $U^+(a, t) = g_a(t)$  and  $U^-(b, t) = g_b(t)$  is

$$\partial_t U^+(t) = \cdots + \frac{s_a}{\Sigma_{11}} [g_a(t) - U^+(t)] \quad \text{at } r = a, \quad (2.65)$$

$$\partial_t U^-(t) = \cdots + \frac{s_b}{\Sigma_{nn}} [g_b(t) - U^-(t)] \quad \text{at } r = b, \quad (2.66)$$

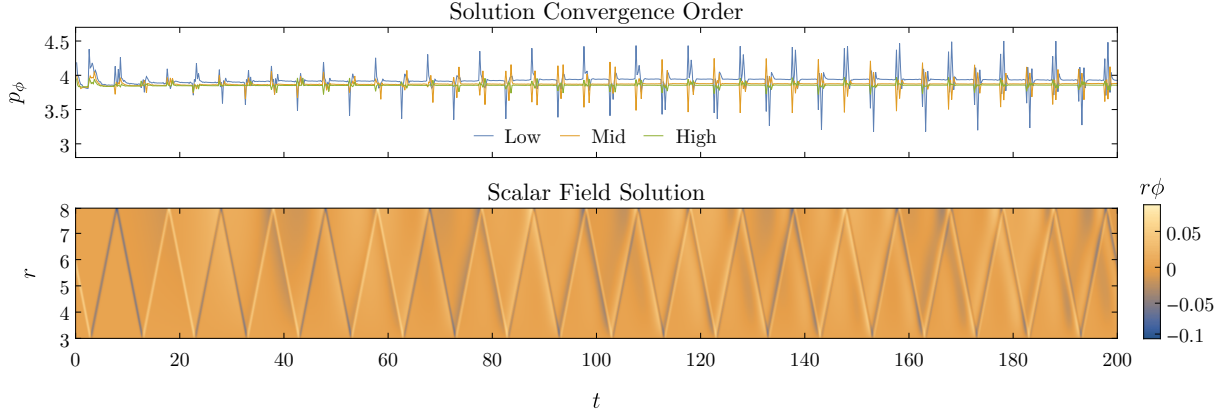


Figure 2.1: Convergence and solution for the flat spherical wave equation. At the top, the solution convergence order settles to about 4<sup>th</sup> order even at coarse resolutions, and deviates only when a reflection occurs where the error is dominated by the boundary region accurate to 3<sup>rd</sup> order. At the bottom we see the wave solution in the  $r$ - $t$  plane, where the pulse travels in straight lines since  $c_\pm = \pm 1$ .

with strengths  $s_a$  and  $s_b$  which dictate the exponential decay scale [29]. One can show that for proper SBP energy conservation, in the context of the wave equation on a static background, the strengths must be equal to the magnitude of the incoming characteristic speeds [30]. At the left boundary we have  $s_a \rightarrow c_+$  and at the right boundary we have  $s_b \rightarrow -c_-$ . In the case of the wave equation around a static background black hole in Kerr-Schild coordinates, we have  $s_b = 1$  and  $0 < s_a < 1$  where  $s_a = 0$  when  $a = 2M_0$  as the boundary is then placed exactly on the horizon, where BCs are not to be imposed anyway since there are no longer any incoming characteristics into the domain at  $r = a$ .

### 2.5.3 Numerical Dissipation

To stabilize nonlinear evolution it is common to add numerical dissipation, ensuring that high frequency noise does not destabilize the evolution. We use the  $A_6$  numerical dissipation operator that applies to the  $D_{6-3}$  operator defined in [59], and it is added to the right hand side of the evolution equations as

$$\partial_t \vec{U} = \dots + \frac{\epsilon}{2^6} A_6 \vec{U}. \quad (2.67)$$

where  $\epsilon > 0$  is the amount of dissipation, which is usually chosen to be of order unity. The coefficients of both operators  $D_{6-3}$  and  $A_6$  can be found in [59].

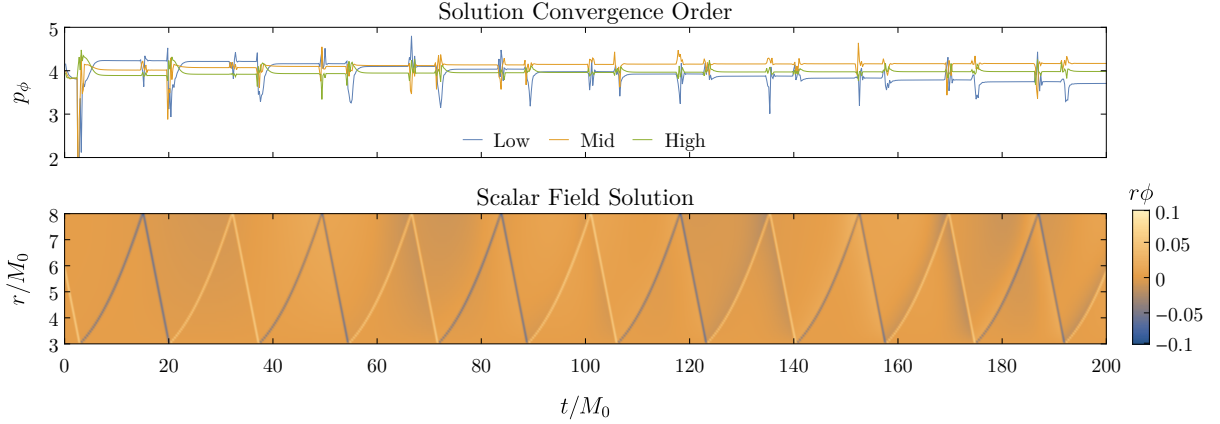


Figure 2.2: Convergence and solution for the static Schwarzschild background wave equation in Kerr-Schild coordinates. At the top, the solution convergence order settles to about 4<sup>th</sup> order as the resolution is increased, deviating when a reflection occurs where the error is dominated by the boundary region accurate to 3<sup>rd</sup> order. At the bottom we see the wave solution in the  $r$ - $t$  plane, where it is apparent that a pulse propagating in the  $-r$  direction has a constant characteristic speed while one traveling in the  $+r$  direction appears to accelerate along curves.

## 2.6 Results

First, to demonstrate long term stability and energy conservation of this framework, an IBVP with two distinct reflection boundaries, one of Dirichlet type and one of Neumann type, will be demonstrated in several situations. Then we will investigate situations where the boundary  $r = a$  is brought very close to the horizon of the black hole. Finally, we discuss the movement of the apparent horizon and situations where the initial pulse can reflect without the apparent horizon moving into the domain.

### 2.6.1 Enclosed Reflecting Boundary Problems

Here we consider several enclosed reflecting boundary problems. These problems involve an initial pulse and BCs of either Dirichlet or Neumann type so that energy is conserved in the continuum limit. We consider three situations for this type of problem, first a Minkowski spherical wave equation, second a static background Schwarzschild black hole in Kerr-Schild coordinates, and third the fully dynamic problem around a black hole. In all of these examples, the initial conditions and evolutions are kept as similar as possible to aid in a direct comparison.

Here, we consider a spatial domain  $r \in [3, 8]M_0$  and a temporal domain  $t \in [0, 200]M_0$ . As the mass  $M_0$  is not relevant in Minkowski space, we simply take  $r \in [3, 8]$  and  $t \in [0, 200]$  in this case. We use a Dirichlet type BC for  $r = a$  (i.e.  $k_a = -1$ ) and a Neumann type BC for  $r = b$  (i.e.  $k_b = 1$ ). For the problems with a black hole, the internal mass is set to  $M_0 = 1$ . The initial pulse follows the model Eq. (2.56) with parameters  $\mu = 6M_0$ ,  $2\sigma = M_0$ , and  $A = 0.05/M_0$ . We use initial condition Eq. (2.57) so that the pulse is initially traveling with speed  $c_- = -1$ .

The time integration is done using 4<sup>th</sup> order Runge-Kutta time stepping, with time step size  $h_t = h/4$ . We also apply the numerical dissipation operator with strength  $\epsilon = 1$  in all cases so that the energy loss is directly comparable to the fully dynamic case.

## Static Minkowski Background

Figure 2.1 depicts the IBVP of the flat spherically symmetric wave equation. To demonstrate the convergence of the solution, we define the solution convergence order:

$$p_\phi^{(i)}(t) = \log_2 \left( \frac{\|\phi^{(i-2)}(t) - \phi^{(i-1)}(t)\|}{\|\phi^{(i-1)}(t) - \phi^{(i)}(t)\|} \right) \quad (2.68)$$

where the  $\phi^{(i)}$  are the solutions obtained with a certain grid spacing  $h^{(i)}$  and where the  $\ell_2$  norm is defined for a grid function  $f$  as

$$\begin{aligned} \|f\|^2 &= \int_a^b f^2 \sqrt{\gamma} \, dr, \\ \|f\|^2 &\approx \|f^{(i)}\|^2 = (f^{(i)})^T W f^{(i)}. \end{aligned} \quad (2.69)$$

We use  $h^{(i)} = h^{(i-1)}/2$  as the resolution is doubled each run. Five runs were conducted starting at  $h^{(1)} = 0.02M_0$ . This leaves three subsets of resolutions to calculate the solution convergence order  $p_\phi^{(i)}$ , referred to as Low ( $i = 3$ ), Mid ( $i = 4$ ), and High ( $i = 5$ ). The  $D_{6-3}$  SBP operator coupled with 4<sup>th</sup> order Runge-Kutta time stepping demonstrates very consistent 4<sup>th</sup> order convergence in this case. Since the characteristic speeds here are  $c_\pm = \pm 1$ , the pulse follows a straight line in the  $r$ - $t$  plane and returns back to  $r = 6$  at precisely  $t = 200$ .

## Static Schwarzschild Background

Figure 2.2 depicts the numerical solution to the IBVP with a static Schwarzschild background in Kerr-Schild coordinates. The same five resolutions are used to obtain the Low,

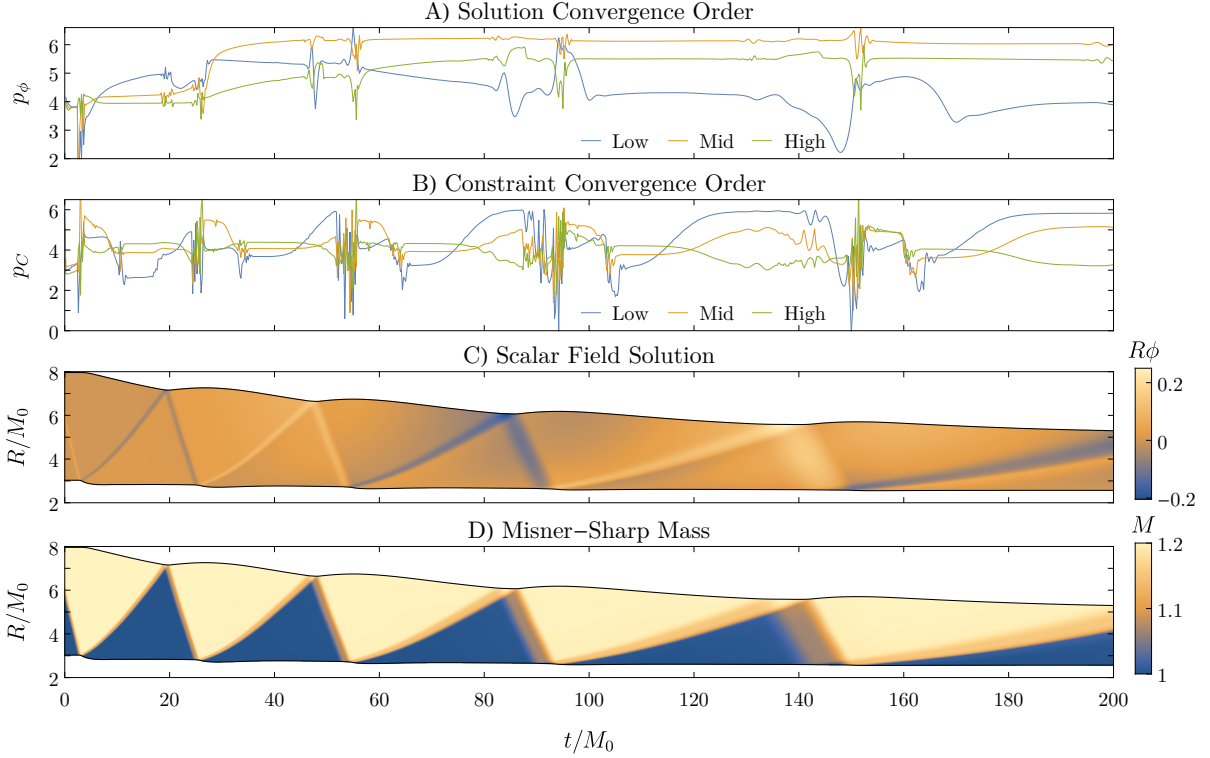


Figure 2.3: Convergence and solution for the fully dynamic IBVP. Plot A) shows the solution convergence order that starts near 4<sup>th</sup> order but changes dramatically as the solution becomes more dependent on boundary interactions and the solution errors move out of phase with each other. Plot B) shows the constraint convergence order slowly settles to about 4<sup>th</sup> order as the resolution is increased. Plot C) shows the scalar field solution shown as a function of the areal radius  $R = \sqrt{\gamma_{\theta\theta}}$  over coordinate time  $t$ . It is apparent that over the course of the evolution, the inner boundary falls toward the horizon by  $\sim 0.5M_0$  and the outer boundary by  $\sim 2.7M_0$ . The pulse also appears to disperse much more than in Fig. 2.2, due to the variation of  $c_{\pm}$  as the Misner-Sharp mass  $M(r)$  changes across the pulse width. Plot D) shows the Misner-Sharp mass in the same  $R$ - $t$  plane, demonstrating the coupling to gravity.

Mid, and High convergence order plots, which shows once again consistent 4<sup>th</sup> order convergence as the resolution is increased. Since the characteristic speeds here are  $c_- = -1$  and  $c_+ = (r - 2M_0)/(r + 2M_0)$ , pulses traveling in the  $-r$  direction follow straight lines in the  $r$ - $t$  plane and stay the same width, but pulses traveling in the  $+r$  direction appear to accelerate along curves and have a characteristic speed that varies across the pulse, so the width increases as the pulse propagates in the  $+r$  direction.

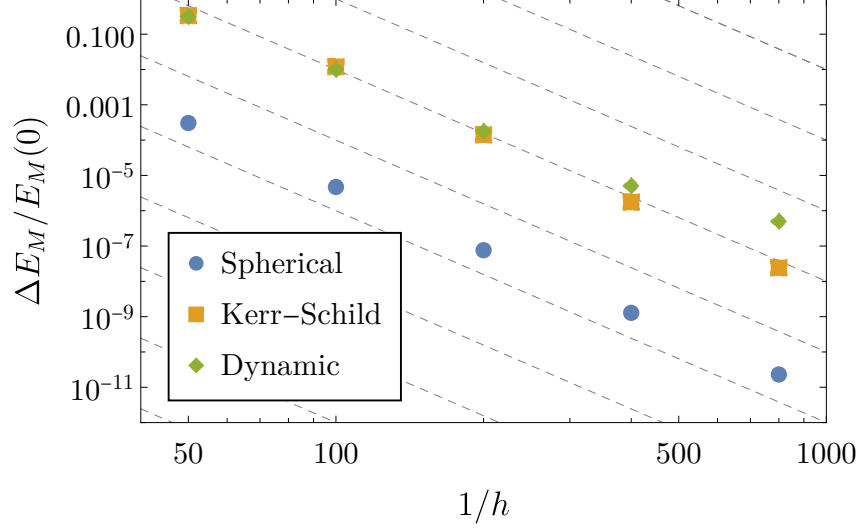


Figure 2.4: Energy loss for various resolutions of the three enclosed boundary scenarios. Here,  $\Delta E_M = E_M(0) - E_M(200)$  and dashed lines are  $\propto h^6$ . The static background cases converge to exact conservation at 6<sup>th</sup> order. The dynamic case appears to diverge from this power law at the highest resolutions.

## Dynamic Schwarzschild Background

Here we demonstrate a fully dynamic IBVP, where the scalar pulse is coupled to gravity. Along with the solution convergence order, we also define the constraint convergence order

$$p_C^{(k)} = \log_2 \left( \frac{\|C_{\text{tot}}^{(k-1)}\|}{\|C_{\text{tot}}^{(k)}\|} \right), \quad (2.70)$$

where the norm of the constraints is defined as

$$\|C_{\text{tot}}\|^2 \equiv \int_a^b (C^2 + \gamma^{ij} C_i C_j) \sqrt{\gamma} dr \quad (2.71)$$

$$\begin{aligned} \|C_{\text{tot}}\|^2 &\approx \|C_{\text{tot}}^{(k)}\|^2 \\ &\equiv (C^{(k)})^T W C^{(k)} + (C_r^{(k)})^T W (C^r)^{(k)} \end{aligned} \quad (2.72)$$

This somewhat simpler definition for the constraint convergence order is possible because we know the exact solution (i.e.  $C = C_r = 0$ ) whereas we don't necessarily know the exact solution for the scalar field  $\phi$ .

We use total reflection BCs on the scalar field Eqns. (2.40) and (2.41) with  $k_a = -1$  and  $k_b = +1$ . We use angular BCs Eqns. (2.42) and (2.43) with  $M(a) = M_0 = 1$  and  $M(b) = M_{\text{tot}}$  for all time, where the value of  $M_{\text{tot}}$  is given from the integration of Eq. (2.58) at the initial time slice and in this case is  $M_{\text{tot}} \sim 1.18M_0$ . And finally, we use radial BCs Eqns. (2.51) and (2.52).

The results are plotted in Figure 2.3. At the initial time slice,  $c_+ = [r - 2M(r)]/[r + 2M(r)]$ , so the outgoing characteristic speed varies across the pulse as in the static background case, but also as  $M(r)$  changes across the pulse width, so there is an additional dispersion due to the coupling to gravity. In this particular gauge,  $\partial_t c_{\pm} = \pm \tilde{\alpha} \partial_t \gamma_{\theta\theta}$ , so the characteristic speeds change proportional to the change in the areal radius,  $R = \sqrt{\gamma_{\theta\theta}}$ . We notice that our choice of BCs causes the boundaries to move inward in  $R$ , making the reflected pulse at the inner boundary move more slowly as time progresses.

In the continuum limit, each of the above IBVPs conserves the energy Eq. (2.39). Figure 2.4 shows that the energy loss at  $t = 200M_0$  in these discrete problems converges to zero at about 6<sup>th</sup> order. Since the strength of the SAT boundary at  $r = a$  depends on the characteristic speed  $c_+$ , it is applied more weakly in the Kerr-Schild and dynamic cases, leading to significantly more energy dissipation at the boundary. This is apparent in Figure 2.4 as the energy decreases about three orders of magnitude more in the Kerr-Schild case than the flat spherical case at  $t = 200M_0$ , although still converges to zero at 6<sup>th</sup> order.

## 2.6.2 Reflections close to the horizon

Black hole echoes are usually discussed in the context of quantum gravity, suggesting that quantum phenomena may result in a reflecting surface. If this is the case, one might expect such a surface to be a distance on the order of the Planck scale away from the horizon (e.g., [60, 49, 50]). To simulate this, one might be interested in applying reflecting BCs very close to the horizon. Although this problem is well-posed in principle, in practice it can be difficult to achieve numerically.

In the context of the static black hole background, if a pulse of width  $w$  is incident on a reflecting surface, the reflected pulse will have width  $\sim w|c_-/c_+|$ , so one should be sure that  $h$  is at least several times smaller than this. There is also usually a significant amount of high frequency noise that propagates at high speed off of the boundary  $r = a$ , which may need to be controlled with numerical dissipation. When  $c_+$  is very small at  $r = a$ , the SATs become very weak and thus lose much more energy, so in order for the discrete problem to conserve energy to a certain tolerance, much more resolution might be required than the naive estimate  $h < w|c_-/c_+|$ .

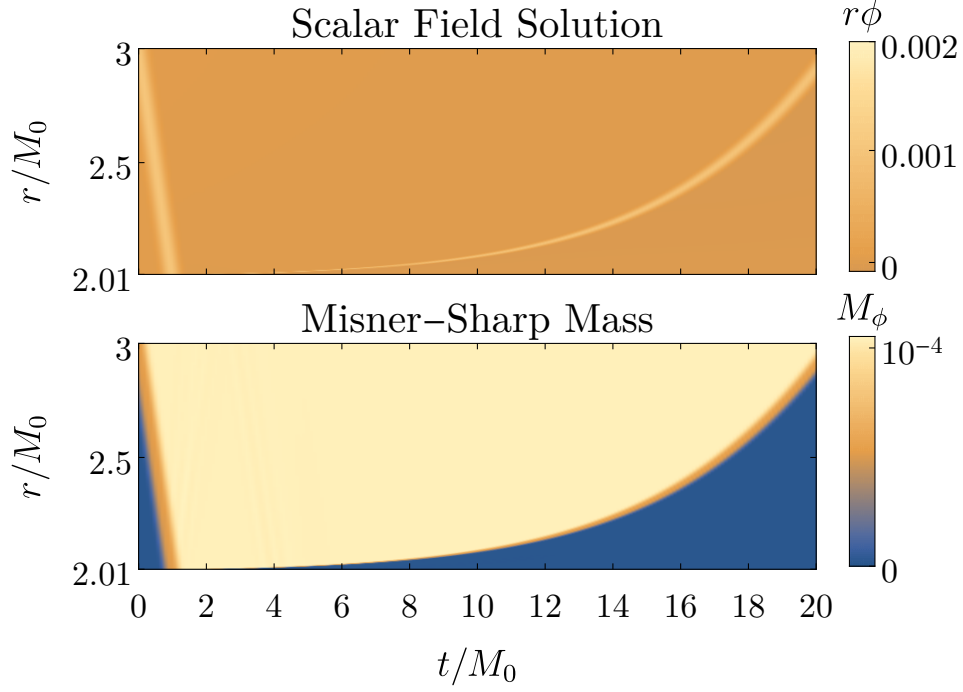


Figure 2.5: A fully dynamic simulation of a scalar pulse incident on a reflection boundary at  $a = 2.01M_0$ . Here the Misner-Sharp mass of the pulse is  $M_\phi = M - M_0$ .

Figure 2.5 depicts a fully dynamic simulation of a scalar pulse incident on a reflecting surface at coordinate radius  $a = 2.01M_0$  with  $k_a = +1$ . For a stellar mass black hole,  $a = 2.01M_0$  is of course far from Planck scale. We mean this as a demonstration of the difficulties one would face in simulating Planck-scale reflections. To achieve a conservation of the Misner-Sharp energy  $E_M$  to within a tolerance of  $\sim 10^{-5}M_0$ , a grid spacing of  $h \sim 6 \times 10^{-5}M_0$  was needed. The parameters of the initial scalar pulse are  $A = 0.001/M_0$ ,  $2\sigma = M_0$ , and  $\mu = 3M_0$ , which results in a total mass  $M_{\text{tot}} \sim (1 + 10^{-4})M_0$  which seems to be about the highest mass allowed (given our gauge and BCs) before the apparent horizon moves into the domain and the boundary can no longer reflect.

### 2.6.3 Apparent Horizons

Finally, as a response to [57], we can study when an apparent horizon moves into the domain of the simulation, making BC Eq. (2.40) ill-defined. In [57], Guo and Mathur argue that for merging equal mass black holes, one should never expect echoes of GWs due to the

formation of an apparent horizon that envelopes the waves. They make the assumption that the waves have a wavelength on the same order of the black hole masses, but any localized wavepacket should contain shorter, as well as longer, wavelengths. If a black hole absorbs a sufficiently localized infalling wavepacket with a total mass  $M_\phi = M_{\text{tot}} - M_0$ , then the apparent horizon should move from  $R = 2M_0$  to  $R = 2M_{\text{tot}}$  as  $t \rightarrow \infty$ . This suggests that a reflecting surface should be located at  $R > 2M_{\text{tot}}$  to ensure that the wavepacket does not become enveloped by a trapped surface. We demonstrate, however, that this estimate can be relaxed for sufficiently wide pulses, and thus the frequency content of a wavepacket plays an important role in whether a reflection can occur.

We consider a domain  $r \in [2.1, 203]M_0$  with the initial pulse location  $\mu = 103M_0$  and vary its width from  $\sigma = 10M_0$  to  $\sigma = 100M_0$ . We consider two situations, one where the boundary  $r = a$  has Neumann type reflective condition  $k_a = +1$ , and one where it has transmitting (or absorbing) condition  $k_a = 0$ . If the mass of the initial pulse  $M_\phi$  is too large, the apparent horizon will move into the domain from its initial position of  $r = 2M_0$  which is initially outside of the domain. We then maximize the mass of the initial pulse by adjusting the amplitude  $A$  to just before this occurs, and plot the results of this maximum mass for the varying initial widths. The transmitting case  $k_a = 0$  demonstrates reflection just from the Schwarzschild potential, a feature that occurs regardless of BCs we apply.

Figure 2.6 shows that the case  $k_a = +1$  (reflective BC) allows a significantly higher maximum mass  $M_\phi$  than the transmitting case  $k_a = 0$  (absorptive BC), which suggests that there is a possibility for low frequency constituents of the incident scalar pulse to reflect near the horizon in a way discernible from reflection due just to the Schwarzschild potential. Indeed, low frequency (or wide) pulses, comparable to the Hawking frequency  $1/(8\pi M_0)$  are also expected to have the largest reflection (from the horizon) based on quantum mechanical arguments [50].

It is important to note that as we have observed previously, our gauge conditions tend to move the boundaries inward, and so the apparent horizon can move into the domain either because it is growing in areal radius, or due to the boundary  $r = a$  shrinking in areal radius. The orange curve in Figure 2.6 should then be thought of as a lower bound that could be higher if the boundary was fixed in areal radius (through a different choice of gauge/BCs).

## 2.7 Conclusion and Future Prospects

In this work, we developed and demonstrated a full initial boundary value problem in numerical relativity in spherical symmetry. In particular, we derived boundary conditions

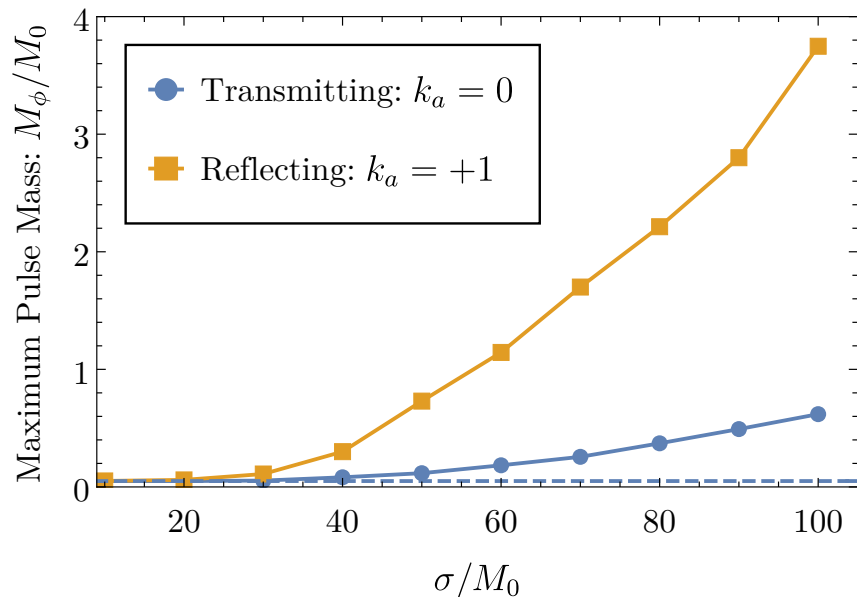


Figure 2.6: Plot of the maximum pulse mass  $M_\phi$  of an initial pulse before the apparent horizon moves into the domain for various widths of the initial pulse. Each case is asymptotic to  $M_\phi = 0.05M_0$  as the width goes to zero ( $\sigma \rightarrow 0$ ), which corresponds to an infinitely sharp pulse with  $a = 2M_{\text{tot}}$ .

(BCs) based on conservation laws involving a quasi-local mass-energy measure, which is the main result of this work. These BCs are general, allowing one to dictate how much mass-energy enters or leaves the domain. We demonstrated how this framework can model black hole echoes, which has mostly been discussed previously either within linear perturbation theory that ignored backreaction or order of magnitude estimates.

However, we only considered a gauge condition where  $\tilde{\alpha}$  and  $\beta^r$  were both time independent. The BC framework presented in Section 2.3 can be applied in the case of a different gauge choice, although the characteristic structure of the evolution equations may change in a non-trivial way. To properly model a black hole echo event, one may want some way of controlling the position of the boundary  $r = a$  relative to the apparent horizon. For example, one might require that the reflection surface remain a constant proper distance from the apparent horizon, so that a pulse can be reflected without the concern that the apparent horizon would move into the domain. Similar conditions are considered in [61, 62], where gauge conditions that ensure the inner boundary of the domain stays just inside the apparent horizon are used, which could be adapted to our case where we want the boundary just *outside* the apparent horizon. We leave a better understanding of how to control the boundary  $r = a$  to future work, that may be prescribed by yet-unknown

quantum gravitational processes.

This BC framework may also be applied in a full 3D simulation. We considered here in spherical symmetry the Misner-Sharp mass as a way to measure the quasi-local mass-energy of the spacetime, but this is not a unique choice. In 3 dimensions, one would need to choose a quasi-local mass-energy measure (e.g. those found in [63]) and derive BCs such that it can be conserved in the same sense as what we have done here. Future work may include a 3D generalization of this framework.

# Chapter 3

## Numerical Relativity in Three Dimensions

### Preface

This chapter contains the work published in [64], titled “Formulating the complete initial boundary value problem in numerical relativity to model black hole echoes”. It has not been altered from its published version other than to adjust some equations to better adhere to the formatting of this thesis and to adjust some figures to better match the relative sizes of fonts. References to ‘we’ in this chapter either refer to the list of authors in [64] (Conner Dailey, Erik Schnetter, and Niayesh Afshordi), or to these authors and the reader.

This work represents a generalization of the previous chapter on spherical symmetry, where completely generic spacetimes without symmetries are appropriately modeled.

### 3.1 Introduction

Recently we described a method for simulating black hole echoes in numerical relativity by imposing reflecting boundary conditions (BCs) near the horizon of a black hole in spherical symmetry [44]. In that work, we defined reflecting BCs on a scalar field based on conservation laws and implemented it using modern numerical methods, including Summation By Parts (SBP) finite differencing operators and BCs applied using Simultaneous Approximation Terms (SATs), to ensure the system remains numerically stable. In an effort to apply this approach to spacetimes with no symmetries, we consider here a generalization to three spatial dimensions.

The motivation to characterize and demonstrate stable initial boundary value problems (IBVPs) in numerical relativity comes from our interest in simulating black hole echoes [50, 13, 51, 16, 52, 53, 49, 15, 54]. Additionally, this is of direct interest to the numerical relativity community in the wake of the first demonstration of Cauchy characteristic matching (CCM) [21], a technique that combines Cauchy evolution and characteristic evolution to provide gravitational wave (GW) scattering feedback to the sources in the Cauchy domain. In [21], it was shown that it is possible to shrink the Cauchy domain while still obtaining accurate gravitational waveforms at null infinity by demonstrating several simulations of black holes perturbed by GWs. Shrinking the Cauchy domain can dramatically save on the computational cost of simulations, as most of this cost comes from the Cauchy evolution. Simulating black hole echoes and evolving CCM necessitate a numerically stable way of evolving dynamical spacetimes with boundaries in the strong gravity regime.

Abandoning spherical symmetry adds a considerable amount of complexity to the BCs and the manner in which they are applied. In [44], we derived and demonstrated reflecting BCs based on the Misner-Sharp mass, which happens to be locally conserved in spherical symmetry. However, in general, local conservation laws do not exist in general relativity. Instead, we have to rely on quasi-local conservation laws to define what it means to reflect gravitational radiation and matter waves. For a review of local and quasi-local conservation laws, see [65]. Although we plan to develop BCs based on controlling the flux of a conserved quasi-local quantity, the focus in this work will be on the adjusted evolution equations, BC framework, and numerical implementation that we develop to make them feasible.

In general, the boundaries of the computational domain can have an arbitrary shape that may not always align with the coordinate directions chosen for the evolution. This is reminiscent of the problem of excision in numerical relativity, where a dynamical black hole interior must be excised so that a physical singularity does not enter the computational domain. Such an excision becomes straightforward with a numerical implementation that

allows for an arbitrarily shaped boundary. If a formulation of numerical relativity with *causal* characteristic speeds is used, no BCs are needed as long as the boundary remains within the apparent horizon of the black hole<sup>1</sup>. In the case where the boundary is *outside* of the apparent horizon, BCs are needed, and their numerical implementation becomes critical to the numerical stability of the simulation. We shall rely on modern methods to ensure that the simulation remains numerically stable for all time. These methods include:

- SBP finite differencing operators for embedded boundaries
- SAT (or weakly implemented) BCs
- Symmetric hyperbolic formulations of numerical relativity, with an approximately conserved energy estimate

In [44], we used the Einstein-Christoffel formulation, as it is one of the few well-tested symmetric hyperbolic formulations of numerical relativity [37]. However, in order to cast the evolution equations into an SBP scheme, we required a formulation more akin to the generalized harmonic (GH) formulation [35, 36, 34, 41, 66], which we consider here instead. Taking care that the energy estimate that comes from symmetric hyperbolicity is conserved in the sense of SBP can ensure that the energy estimate is bounded, and thus the simulation is, in principle, stable for all time (at least for linear short-wavelength perturbations). The principal goal of this work is to adapt the first order system introduced in [41] into a proper SBP-SAT scheme, which will require critical differences in the way the equations are evolved and the BCs are applied.

In Section 3.2, we define covariant SBP methods with the wave equation as an example. In Section 3.3 we present our altered GH first order system and describe its SBP energy estimates. In Section 3.4, we describe how we set up initial conditions and in Section 3.5 we present our BC framework. In Section 3.6 we describe two embedded boundary SBP methods and chose one to implement and adapt to the GH first order system. Finally, in Section 3.7 we present our results where we consider several IBVPs involving gravitational wave scattering with boundaries placed inside and just outside of the horizons of spinning and non-spinning black holes.

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<sup>1</sup>Although being inside the apparent horizon is sufficient, it may not be strictly necessary since the apparent horizon world tube is still inside the event horizon.

## 3.2 Covariant Summation By Parts

A popular way to maintain stability in numerical hyperbolic IBVPs is to use finite differencing operators that satisfy summation by parts (SBP). Using SBP operators has been proven to be closely related to the well-posedness and the numerical stability of many conservative problems [29, 30]. The SBP property is usually discussed with respect to flat space and one dimension, defining a discrete analog of traditional integration by parts. Here, we make an effort to generalize the one dimensional covariant version of this property we developed in [44] into a multidimensional approach that is applicable to spacetimes without symmetries.

Consider a scalar field  $\phi$  that satisfies the massless Klein-Gordon equation  $\nabla^\mu \nabla_\mu \phi = 0$ , where  $\nabla_\mu$  is the covariant derivative with respect to the metric  $g_{\mu\nu}$ . This equation can be reduced to a first order system with the definition of two auxiliary variables:  $\Pi \equiv -n^\mu \partial_\mu \phi$  and  $\psi_i \equiv \partial_i \phi$ , where  $n^\mu$  is the timelike future-directed unit normal to the 3-space with metric  $\gamma_{ij}$ . In this work, Greek indices run over space and time, while Latin indices run over space only. If we consider a time independent background metric, we obtain the following system of evolution equations:

$$\partial_t \phi = \beta^i \psi_i - \alpha \Pi, \quad (3.1)$$

$$\partial_t \psi_i + \partial_i (\alpha \Pi - \beta^j \psi_j) = 0, \quad (3.2)$$

$$\partial_t \Pi + \bar{\nabla}_i (\alpha \psi^i - \beta^i \Pi) = 0, \quad (3.3)$$

where  $\bar{\nabla}_i f^i = (\sqrt{\gamma})^{-1} \partial_i (\sqrt{\gamma} f^i)$  is the vector 3-divergence,  $\gamma$  is the determinant of  $\gamma_{ij}$ ,  $\alpha$  is the lapse, and  $\beta^i$  is the shift. In this system, Eq. (3.1) is just the definition of  $\Pi$ , Eq. (3.2) enforces the commutativity of temporal and spatial derivatives, and Eq. (3.3) enforces the massless Klein-Gordon equation. The equations are written so that the left hand side contains the principal part, while the right hand side contains only source terms.

Since a time independent metric necessarily contains a timelike Killing vector  $\xi^\mu$ , the background spacetime is stationary and there exists a conserved current  $J^\mu = T^{\mu\nu} \xi_\nu$ , where  $T_{\mu\nu}$  is the stress-energy tensor. If we define the stationary energy

$$E_s = \frac{1}{2} \int [\alpha (\Pi^2 + \psi_i \psi^i) - 2 \Pi \beta^i \psi_i] dV, \quad (3.4)$$

where  $dV$  is the volume element of the 3-space, we can rewrite the conservation property  $\nabla_\mu J^\mu = 0$  to see that this energy is locally conserved:

$$\partial_t E_s = \oint (\alpha \Pi - \beta^j \psi_j) s_i (\alpha \psi^i - \beta^i \Pi) dS. \quad (3.5)$$

The right hand side describes the flux through a boundary surface  $S$  and  $s_i$  is the spacelike unit normal to that boundary. If we define the scalar  $u \equiv \alpha\Pi - \beta^j\psi_j$  and the vector  $v^i \equiv \alpha\psi^i - \beta^i\Pi$ , we can write an “integration by parts” rule with respect to this conservation law:

$$\int u \bar{\nabla}_i v^i dV + \int (\partial_i u) v^i dV = \oint u s_i v^i dS. \quad (3.6)$$

If we instead define a vector field  $F^i \equiv uv^i$ , we see that this is nothing more than the covariant divergence theorem:

$$\int \bar{\nabla}_i F^i dV = \oint s_i F^i dS. \quad (3.7)$$

Now we consider functions discretely sampled on a grid. A traditional one dimensional SBP derivative operator  $D$ , along with its norm operator  $\Sigma$ , satisfy

$$u^T \Sigma D v + (D u)^T \Sigma v = u^T B v, \quad (3.8)$$

where  $B = \text{diag}(-1, 0, \dots, 0, 1)$ , for any two functions  $u$  and  $v$  sampled on a grid. In dimensions greater than one,  $v$  will take the role of a vector valued function<sup>2</sup>. With a few alterations, the covariant version of this property in 3D can be written as

$$u^T W \mathcal{D}_i v^i + (D_i u)^T W v^i = u^T S_i v^i. \quad (3.9)$$

Here, the operator  $\mathcal{D}_i \equiv \Gamma^{-1} D_i \Gamma$  approximates the 3-divergence, the operator  $D_i$  approximates the scalar gradient, and  $W \equiv \Sigma \mathcal{W}$  is the covariant norm operator that approximates 3-volume integration, where operator  $\mathcal{W}$  is a diagonal matrix with the values of  $\sqrt{\gamma}$  injected along that diagonal. Finally,  $S_i \equiv B \mathcal{S}_i$  is the boundary operator that approximates covariant surface integrals, where  $\mathcal{S}_i$  are diagonal matrices with the values of  $s_i \sqrt{\sigma}$  injected along those diagonals and  $\sigma$  is the determinant of the metric on the 2-surface of the boundary. This is to be directly compared with the continuous version Eq. (3.6). This is not the only way to think about the covariant SBP energy estimate; one might include an arbitrary positive definite symmetrizer for example, but we find this way particularly elegant.

The SBP scheme we employ uses finite differencing operators that act on each of the variables  $u$  and  $v^i$ , as is suggested by the left hand side of Eqs. (3.2) and (3.3), which is in contrast to expanding the definition of these variables into multiple terms using the product

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<sup>2</sup>The boundary operator has this form if grid values on the boundary are included. It has a different interpolating/extrapolating form if this is not the case (see for example [67]).

rule of continuous calculus, as is common in numerical techniques. This is important for maintaining SBP, as discrete operators generally do not obey the product rule [68]. The evolution equations are then reminiscent of the flux-conservative form common in hydrodynamic systems.

The SBP formalism defined by Eq. (3.9) is completed by using an SBP operator in place of  $D_i$ . Although we will focus on finite differencing based SBP operators in this work, in principle SBP operators based on other methods, such as spectral methods, can complete this SBP formalism as well. The system of equations we used as an example in this section happens to have a local conservation law on which we can base the SBP property. This is not true in general for an arbitrary system of equations, like Einstein's equations. Instead, as long as the system of equations can be shown to be symmetric hyperbolic, there exists an energy estimate with respect to the principal part of the system [27]. It is this energy estimate that we aim our SBP method to preserve.

### 3.3 The Generalized Harmonic First Order System

As first introduced by [35, 36], the Einstein field equations can be cast as a symmetric hyperbolic system by introducing a Generalized Harmonic (GH) gauge. Many successful numerical relativity simulations have since been based on this formulation (for example [38, 39, 40]). The GH evolution equations can also be written as a symmetric hyperbolic first order system of equations [41]. To this end, a set of gauge functions  $H_\mu$  are defined on a Lorentzian spacetime with metric  $g_{\mu\nu}$  and coordinates  $x^\mu$ :

$$H_\mu(x^\alpha) = -g_{\mu\sigma}\nabla_\nu\nabla^\nu x^\sigma = g^{\alpha\beta}\Gamma_{\mu\alpha\beta} \equiv \Gamma_\mu, \quad (3.10)$$

where  $\Gamma_{\alpha\mu\nu}$  is the connection with respect to the metric  $g_{\mu\nu}$ . For  $H_\mu = 0$ , this becomes the harmonic coordinate condition, but for an arbitrary set of spacetime functions, any gauge condition can be specified in principle. This set of gauge conditions can also be expressed as evolution equations for the lapse and shift:

$$\partial_t\alpha - \beta^i\partial_i\alpha = \alpha^2(n^\mu H_\mu - K), \quad (3.11)$$

$$\partial_t\beta^i - \beta^j\partial_j\beta^i = \alpha^2\gamma^{ij}(\gamma^{kl}\Gamma_{jkl} - H_j - \partial_j\ln\alpha), \quad (3.12)$$

where  $K = \nabla^\mu n_\mu$  is the trace of the extrinsic curvature  $K_{\mu\nu}$ .

It has also been demonstrated that the evolution of  $H_\mu$  can be achieved alongside the Einstein field equations [38, 39], where a wave-like evolution scheme is adopted. The

symmetric hyperbolicity of the GH evolution equations can be destroyed with an arbitrary evolution scheme for  $H_\mu$ . By picking an evolution scheme of second order, such as a wave operator (evolved as a first order system of equations) the symmetric hyperbolicity of the GH evolution equations is maintained, as the principal part is not altered. For simplicity, in this work we will focus on a function specification of  $H_\mu(x^\nu)$ , where we effectively use the gauge condition  $\partial_t H_\mu = 0$ .

With the two auxiliary definitions  $P_{\mu\nu} \equiv -n^\alpha \partial_\alpha g_{\mu\nu}$  and  $d_{i\mu\nu} \equiv \partial_i g_{\mu\nu}$ , we can write the symmetric hyperbolic GH evolution system as

$$\partial_t g_{\mu\nu} = \beta^i d_{i\mu\nu} - \alpha P_{\mu\nu}, \quad (3.13)$$

$$\partial_t d_{i\mu\nu} + \partial_i(\alpha P_{\mu\nu} - \beta^j d_{j\mu\nu}) = 0, \quad (3.14)$$

$$\begin{aligned} \partial_t P_{\mu\nu} + \bar{\nabla}_i(\alpha d^i_{\mu\nu} - \beta^i P_{\mu\nu}) = & -(\partial_t \ln \sqrt{\gamma}) P_{\mu\nu} + 2\alpha \partial_{(\mu} H_{\nu)} - 2\alpha H_\sigma \Gamma^\sigma_{\mu\nu} - \alpha \Gamma^\sigma_{\sigma} \partial_\sigma g_{\mu\nu} \\ & + 2\alpha g^{\epsilon\sigma} g^{\lambda\rho} (\partial_\lambda g_{\epsilon\mu} \partial_\rho g_{\sigma\nu} - \Gamma_{\mu\epsilon\lambda} \Gamma_{\nu\sigma\rho}), \end{aligned} \quad (3.15)$$

where the operator  $\bar{\nabla}_i$  acts still as a *vector* divergence so that  $\bar{\nabla}_i f^i_{\mu\nu} \equiv (\sqrt{\gamma})^{-1} \partial_i (\sqrt{\gamma} f^i_{\mu\nu})$ . In this system, Eq. (3.13) is just the definition of  $P_{\mu\nu}$ , Eq. (3.14) enforces the commutativity of temporal and spatial derivatives, and Eq. (3.15) enforces the vacuum Einstein field equations.

This system of first order equations has state vector  $\vec{U} = (g_{\mu\nu}, d_{i\mu\nu}, P_{\mu\nu})$ . It is understood that where Christoffel symbols, first-order metric derivatives, lapse, and shift appear in the evolution equations, they stand for elements of the state vector according to their definitions. For the Christoffel symbols we have

$$2\Gamma_{\alpha\mu\nu} = \partial_\mu g_{\alpha\nu} + \partial_\nu g_{\alpha\mu} - \partial_\alpha g_{\mu\nu}, \quad (3.16)$$

and all first order metric derivatives are defined via the state vector with

$$\partial_t g_{\mu\nu} = \beta^i d_{i\mu\nu} - \alpha P_{\mu\nu}, \quad (3.17)$$

$$\partial_i g_{\mu\nu} = d_{i\mu\nu}. \quad (3.18)$$

The time derivative of the 3-metric determinant is expressed as

$$\partial_t \ln \sqrt{\gamma} = \frac{1}{2} \gamma^{ij} \partial_t \gamma_{ij} = \frac{1}{2} \gamma^{ij} (\beta^k d_{kij} - \alpha P_{ij}), \quad (3.19)$$

and the lapse and shift are set via the inverse metric components

$$\alpha^2 = (-g^{tt})^{-1}, \quad \beta^i = \alpha^2 g^{ti}. \quad (3.20)$$

This system is very similar to that defined originally by [41], except we have altered the principal part in the same sense as suggested by Section 3.2.

Since the first order GH formulation is symmetric hyperbolic, it admits an energy estimate with respect to the principal part of the system [27, 41]:

$$E_g = \frac{1}{2} \int m^{\mu\nu} m^{\epsilon\sigma} \left[ \alpha (P_{\mu\epsilon} P_{\nu\sigma} + d_{\mu\epsilon}^i d_{i\nu\sigma}) - 2\beta^i P_{\mu\epsilon} d_{i\nu\sigma} \right] dV, \quad (3.21)$$

where  $m^{\mu\nu}$  is any positive definite metric (we use  $m^{\mu\nu} = n^\mu n^\nu + \gamma^{\mu\nu}$ ). This energy is locally conserved

$$\partial_t E_g \sim \oint m^{\mu\nu} m^{\epsilon\sigma} (\alpha P_{\mu\epsilon} - \beta^j d_{j\mu\epsilon}) s_i (\alpha d_{\nu\sigma}^i - \beta^i P_{\nu\sigma}) dS, \quad (3.22)$$

if we ignore the source terms on the right hand side of GH evolution equations. By writing these equations as we have, and defining  $u_{\mu\nu} \equiv \alpha P_{\mu\nu} - \beta^j d_{j\mu\nu}$  and  $v_{\mu\nu}^i \equiv \alpha d_{\mu\nu}^i - \beta^i P_{\mu\nu}$ , we can write an “integration by parts” rule for this system, keeping only terms from the principal part:

$$\int m^{\mu\nu} m^{\epsilon\sigma} [u_{\mu\epsilon} \bar{\nabla}_i v_{\nu\sigma}^i + (\partial_i u_{\mu\epsilon}) v_{\nu\sigma}^i] dV \sim \oint m^{\mu\nu} m^{\epsilon\sigma} u_{\mu\epsilon} s_i v_{\nu\sigma}^i dS. \quad (3.23)$$

Just as in Section (3.2), we endeavor to write a discrete analog of this property. We sample the functions  $u_{\mu\nu}$  and  $v_{\mu\nu}^i$  to a grid and obtain

$$(u_{\mu\nu})^T W^{\mu\nu\alpha\beta} \mathcal{D}_i v_{\alpha\beta}^i + (D_i u_{\mu\nu})^T W^{\mu\nu\alpha\beta} v_{\alpha\beta}^i = (u_{\mu\nu})^T S_i^{\mu\nu\alpha\beta} v_{\alpha\beta}^i. \quad (3.24)$$

The operators  $\mathcal{D}_i$  and  $D_i$  act the same as in Section (3.2), but the covariant norm operator is  $W^{\mu\nu\alpha\beta} \equiv \Sigma \mathcal{W}^{\mu\nu\alpha\beta}$  where  $\mathcal{W}^{\mu\nu\alpha\beta}$  is a diagonal matrix with the values of  $\sqrt{\gamma} m^{\mu\alpha} m^{\nu\beta}$  injected along that diagonal. Finally,  $S_i^{\mu\nu\alpha\beta} = B \mathcal{S}_i^{\mu\nu\alpha\beta}$  is the boundary operator for this system, where  $\mathcal{S}_i^{\mu\nu\alpha\beta}$  are diagonal matrices with the values of  $s_i \sqrt{\sigma} m^{\mu\alpha} m^{\nu\beta}$  injected along those diagonals. This allows for the direct application of SBP methods to this system of evolution equations if the substitution  $\bar{\nabla}_i \rightarrow \mathcal{D}_i$  and  $\partial_i \rightarrow D_i$  is made with an appropriate SBP derivative operator.

The GH formulation introduces the set of gauge constraints  $\mathcal{C}_\alpha \equiv g^{\mu\nu} \Gamma_{\alpha\mu\nu} - H_\alpha$  and the first order reduction introduces the set of spatial derivative constraints  $\mathcal{C}_{i\mu\nu} \equiv D_i g_{\mu\nu} - d_{i\mu\nu}$ . To ensure that these constraints do not grow during the evolution, constraint damping terms are added to the right hand side of the evolution equations [41]:

$$\partial_t d_{i\mu\nu} = \cdots + \gamma_2 \alpha \mathcal{C}_{i\mu\nu}, \quad (3.25)$$

$$\partial_t P_{\mu\nu} = \cdots - \gamma_2 \beta^i \mathcal{C}_{i\mu\nu} + \gamma_0 \alpha (2n_{(\mu} \mathcal{C}_{\nu)} - g_{\mu\nu} n^\epsilon \mathcal{C}_\epsilon), \quad (3.26)$$

which results in exponential damping of constraint violations as long as the rate parameters  $\gamma_{0,2}$  are positive. The time derivatives of the gauge constraints  $(\partial_t \mathcal{C}_\alpha)$  can be shown to effectively replace the Einstein constraints  $\mathcal{M}^\nu = n_\mu G^{\mu\nu}$  [41, 66], where  $G^{\mu\nu}$  is the Einstein tensor, which allows us to infer that  $\mathcal{M}^\mu = 0$  from static behavior in  $\mathcal{C}^\mu$ . In fact, if one can show  $\mathcal{C}_\mu = \partial_i \mathcal{C}_\mu = 0$ , then  $\partial_t \mathcal{C}_\mu = 2\alpha \mathcal{M}_\mu$ .

### 3.4 Initial Conditions

Given a completely arbitrary metric on the initial hypersurface  $g_{\mu\nu}(t=0) = g_{\mu\nu}^{\text{init}}$ , we aim to set up initial conditions for the rest of the state-vector while controlling the set of constraints defined above. We can easily control the initial values of the constraints  $\mathcal{C}_{i\mu\nu}$  by setting

$$d_{i\mu\nu}^{\text{init}} = D_i g_{\mu\nu} - \mathcal{C}_{i\mu\nu}^{\text{init}}, \quad (3.27)$$

for an arbitrary set of functions  $\mathcal{C}_{i\mu\nu}^{\text{init}}$ . Next, we can control the initial values of  $\mathcal{C}_\alpha$  by setting 4 of the initial components of  $P_{\mu\nu}$ . The definition of  $\mathcal{C}_\alpha$  gives

$$\mathcal{C}_\alpha = \left( n^{(\mu} \delta^{\nu)}_\alpha - \frac{1}{2} g^{\mu\nu} n_\alpha \right) P_{\mu\nu} + \left( \gamma^{i(\mu} \delta^{\nu)}_\alpha - \frac{1}{2} g^{\mu\nu} \gamma^i_\alpha \right) d_{i\mu\nu} - H_\alpha. \quad (3.28)$$

We then define two projection operators that transfer between components of symmetric second rank tensors:

$$\delta_{(\mu}^{(\alpha} \delta_{\nu)}^{\beta)} = A_{\mu\nu}^{\alpha\beta} + B_{\mu\nu}^{\alpha\beta}. \quad (3.29)$$

The operator  $A_{\mu\nu}^{\alpha\beta}$  acts to pick out the 4 degrees of freedom in  $P_{\mu\nu}$  responsible for the values of  $\mathcal{C}_\alpha$ :

$$A_{\mu\nu}^{\alpha\beta} \equiv n_\mu n_\nu n^\alpha n^\beta - 2n_{(\mu} \gamma_{\nu)}^{(\alpha} n^{\beta)} + n_\mu n_\nu \gamma^{\alpha\beta}, \quad (3.30)$$

which has a complimentary operator

$$A_{\mu\nu}^{\alpha} \equiv n_{(\mu} \gamma_{\nu)}^{\alpha} - n_\mu n_\nu n^\alpha, \quad (3.31)$$

that satisfies  $A_{\mu\nu}^{\alpha\beta} A_{\alpha\beta}^\epsilon = A_{\mu\nu}^\epsilon$ . Together, they complete the relation

$$A_{\mu\nu}^{\alpha\beta} P_{\alpha\beta}^{\text{init}} = A_{\mu\nu}^\epsilon (2\gamma^{i\alpha} d_{i\alpha\epsilon} - g^{\alpha\beta} \gamma_\epsilon^i d_{i\alpha\beta} - 2H_\epsilon - 2\mathcal{C}_\epsilon^{\text{init}}), \quad (3.32)$$

for an arbitrary set of functions  $\mathcal{C}_\epsilon^{\text{init}}(x^i)$ . The other components of  $P_{\mu\nu}^{\text{init}}$  are arbitrary, and can be set however desired with the operator

$$B_{\mu\nu}{}^{\alpha\beta} \equiv \gamma_{(\mu}^{(\alpha} \gamma_{\nu)}^{\beta)} - n_\mu n_\nu \gamma^{\alpha\beta}. \quad (3.33)$$

In principle, these remaining components of  $P_{\mu\nu}$  selected by this operator can be assigned meaning as we will do in a similar way in the next section, but we don't find this necessary for this work. Our choices for the projection operators used here might not be unique.

For most practical applications, the choice to satisfy the constraints on the initial hypersurface (i.e.  $\mathcal{C}_\alpha^{\text{init}} = \mathcal{C}_{i\mu\nu}^{\text{init}} = 0$ ) will be desired, but allowing them to be set arbitrarily is very useful for numerical tests. Setting the values of  $\mathcal{C}_\alpha^{\text{init}} = 0$  does not necessarily imply that the Einstein constraints are satisfied however, as they are effectively controlled with  $\partial_t \mathcal{C}_\alpha^{\text{init}}$ , but with the addition of an appropriate rate of constraint damping, any initial value of  $\partial_t \mathcal{C}_\alpha^{\text{init}}$  will vanish quickly.

## 3.5 Boundary Conditions

The generic method of applying BCs to systems of hyperbolic IBVPs is the method of characteristics. The characteristic modes and speeds are defined based on the eigenvectors and eigenvalues of the principal part of the system (see [23] for a review). Given a boundary hypersurface with purely spatial unit normal  $s^\mu$  orthogonal to  $n^\mu$  pointing out of the computational domain, the characteristic modes for this system are given by <sup>3</sup>

$$U_{\mu\nu}^+ \equiv k^\alpha \partial_\alpha g_{\mu\nu} = -\frac{1}{\sqrt{2}}(P_{\mu\nu} + s^i d_{i\mu\nu}), \quad (3.34)$$

$$U_{\mu\nu}^- \equiv \ell^\alpha \partial_\alpha g_{\mu\nu} = -\frac{1}{\sqrt{2}}(P_{\mu\nu} - s^i d_{i\mu\nu}), \quad (3.35)$$

$$U_{\alpha\mu\nu}^\perp \equiv \sigma_\alpha{}^\beta \partial_\beta g_{\mu\nu} = \sigma_\alpha{}^i d_{i\mu\nu}. \quad (3.36)$$

The characteristic modes are only unique up to a constant multiplicative factor, and we find it convenient to normalize them such that they are simply the derivatives in the direction of the outgoing null vector  $\ell^\mu = (n^\mu + s^\mu)/\sqrt{2}$ , the ingoing null vector  $k^\mu = (n^\mu - s^\mu)/\sqrt{2}$ , and the metric on the 2-surface of the boundary  $\sigma_{\mu\nu} = g_{\mu\nu} + 2\ell_{(\mu} k_{\nu)}$ . The characteristics  $U_{\mu\nu}^\pm$

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<sup>3</sup>Technically, with the addition of the derivative constraint damping, the definitions of  $U_{\mu\nu}^\pm$  should contain an additional term  $\gamma_2 g_{\mu\nu}$ , but for simplicity, we considered a characteristic decomposition based on first derivatives of the metric only, and we found that this works well. The formulas presented in this work can be cast in terms of the proper characteristics  $\tilde{U}_{\mu\nu}^\pm$  with the relationship  $\tilde{U}_{\mu\nu}^\pm = U_{\mu\nu}^\pm + \gamma_2 g_{\mu\nu}/\sqrt{2}$ .

travel along the light cone with coordinate speed  $c_{\pm} = \pm\alpha - s_i\beta^i$ . The characteristics  $U_{\alpha\mu\nu}^{\perp}$  travel along  $n^{\mu}$  with coordinate speed  $c_{\perp} = -s_i\beta^i$ . The method of characteristics dictates that all of the modes with a characteristic speed negative in value (i.e. propagating into the computational domain) require BCs.

The characteristic  $U_{\mu\nu}^{-}$  at a point on the boundary is always incoming unless the boundary worldtube is not timelike there (such as if it is within an apparent horizon), so we assign to it the physical incoming degrees of freedom, and we will replace these components with our BCs (i.e.  $U_{\mu\nu}^{-} \rightarrow U_{\mu\nu}^{-\text{BC}}$ ). If the characteristic  $U_{\alpha\mu\nu}^{\perp}$  is incoming, we set it by demanding the vanishing of the derivative constraints  $\mathcal{C}_{i\mu\nu} = 0$ . If  $U_{\mu\nu}^{-}$  is the only incoming characteristic for example, the values of the state vector can be reconstructed on the boundary as

$$P_{\mu\nu}^{\text{BC}} = -\frac{1}{\sqrt{2}}(U_{\mu\nu}^{+} + U_{\mu\nu}^{-\text{BC}}), \quad (3.37)$$

$$d_{i\mu\nu}^{\text{BC}} = U_{i\mu\nu}^{\perp} - \ell_i U_{\mu\nu}^{+} - k_i U_{\mu\nu}^{-\text{BC}}. \quad (3.38)$$

We still need to understand which of the components of  $U_{\mu\nu}^{-\text{BC}}$  affect which degrees of freedom of the metric itself. Here, we follow and generalize the component projection formalism discussed in [41].

We introduce the following decomposition of the identity operator that transfers between components of symmetric second rank tensors:

$$\delta_{(\mu}^{(\alpha} \delta_{\nu)}^{\beta)} = C_{\mu\nu}^{\alpha\beta} + P_{\mu\nu}^{\alpha\beta} + G_{\mu\nu}^{\alpha\beta}. \quad (3.39)$$

Each of these operators has a clear interpretation as to what incoming degrees of freedom in the metric they control, which are elaborated in the following subsections.

### 3.5.1 Constraint Controlling BCs

Four of the components of  $U_{\mu\nu}^{-\text{BC}}$  can be used to control the values of the gauge constraints  $\mathcal{C}_{\alpha}$  on the boundary. The operator

$$C_{\mu\nu}^{\alpha\beta} \equiv \frac{1}{2}\sigma_{\mu\nu}\sigma^{\alpha\beta} - 2\ell_{(\mu}\sigma_{\nu)}^{(\alpha}k^{\beta)} + \ell_{\mu}\ell_{\nu}k^{\alpha}k^{\beta}, \quad (3.40)$$

picks out these components. There is also a complementary operator

$$C_{\mu\nu}^{\alpha} \equiv \ell_{(\mu}\sigma_{\nu)}^{\alpha} - \frac{1}{2}\sigma_{\mu\nu}\ell^{\alpha} - \frac{1}{2}\ell_{\mu}\ell_{\nu}k^{\alpha}, \quad (3.41)$$

that satisfies  $C_{\mu\nu}{}^{\alpha\beta}C_{\alpha\beta}{}^{\epsilon} = C_{\mu\nu}{}^{\epsilon}$ . The form of these operators (originally written in [41]), comes directly from the definition of the gauge constraints ( $\mathcal{C}_\alpha = g^{\mu\nu}\Gamma_{\alpha\mu\nu} - H_\alpha$ ). This definition is equivalent to

$$C_{\mu\nu}{}^{\alpha\beta}U_{\alpha\beta}^{-\text{BC}} = C_{\mu\nu}{}^{\epsilon}\left(2\ell^\alpha U_{\alpha\epsilon}^+ - \ell_\epsilon g^{\alpha\beta}U_{\alpha\beta}^+ + g^{\alpha\beta}U_{\epsilon\alpha\beta}^\perp - 2g^{\alpha\beta}U_{\alpha\beta\epsilon}^\perp + 2H_\epsilon + 2\mathcal{C}_\epsilon^{\text{BC}}\right), \quad (3.42)$$

where we have allowed for some arbitrary functions  $\mathcal{C}_\mu^{\text{BC}}(x^\alpha)$ . In this fashion, the values of  $\mathcal{C}_\alpha$  on the boundary are specified by the BCs desired.

### 3.5.2 Gravitational Wave Controlling BCs

The operator  $P_{\mu\nu}{}^{\alpha\beta}$  is the traceless part of the projection onto the 2 dimensional manifold of the boundary

$$P_{\mu\nu}{}^{\alpha\beta} \equiv \sigma_{(\mu}{}^{(\alpha} \sigma_{\nu)}{}^{\beta)} - \frac{1}{2}\sigma_{\mu\nu}\sigma^{\alpha\beta}, \quad (3.43)$$

and controls the 2 degrees of freedom that dictate physical incoming GWs [41]. We can inject a GW model through the boundary by picking an arbitrary model  $h_{\mu\nu}^{\text{BC}}$  and setting it with

$$P_{\mu\nu}{}^{\alpha\beta}U_{\alpha\beta}^{-\text{BC}} = P_{\mu\nu}{}^{\alpha\beta}h_{\alpha\beta}^{\text{BC}}. \quad (3.44)$$

It was shown in [69] that the object  $P_{\mu\nu}{}^{\alpha\beta}s^i\partial_i U_{\alpha\beta}^-$  is related to the complex Newman-Penrose curvature scalar  $\Psi_0$  ( $\Psi_4$ ) at the outer (inner) boundary. The model  $h_{\alpha\beta}^{\text{BC}}$  can then be thought of as related to a line integral over  $\Psi_0$  or  $\Psi_4$  in the direction  $s^i$  via the gradient theorem. If we decompose the 2-metric into two spatial directions using a set of orthonormal basis vectors  $p^\mu$  and  $q^\mu$  such that  $\sigma_{\mu\nu} = p_\mu p_\nu + q_\mu q_\nu$ , we can see (as expected) that there are only two components of this projection, and they are related to derivatives of  $\sigma_{\mu\nu}$ :

$$(p^\mu p^\nu - q^\mu q^\nu)P_{\mu\nu}{}^{\alpha\beta}U_{\alpha\beta}^- = (p^\mu p^\nu - q^\mu q^\nu)\ell^\alpha \partial_\alpha \sigma_{\mu\nu}, \quad (3.45)$$

$$p^\mu q^\nu P_{\mu\nu}{}^{\alpha\beta}U_{\alpha\beta}^- = p^\mu q^\nu \ell^\alpha \partial_\alpha \sigma_{\mu\nu}. \quad (3.46)$$

The former controls the  $+$  polarization and the latter controls the  $\times$  polarization with respect to these basis vectors.

In principle these components can also be set using an arbitrary function of the outgoing fields

$$h_{\alpha\beta}^{\text{BC}} = h_{\alpha\beta}^{\text{BC}}(U_{\mu\nu}^+, U_{\sigma\mu\nu}^\perp), \quad (3.47)$$

but careful analysis and numerical testing is needed to understand what a specific choice implies about the GWs that would be injected into the computational domain in response to the GWs incident on the boundary itself. One way to do this is to use a conservation law to gain some insight.

Since in 3D general relativity does not have local conservation laws, we can consider instead a class of quasi-local conservation laws [65]. These are called quasi-local because instead of relating the change in a volume integral to the flux through a 2-surface, they relate the change in a 2-surface integral to the flux through a 2-surface, and hence they only depend on the geometry in the neighborhood of the 2-surface. Just as we have done in [44], we can in principle define BCs on GWs that control the flux portion of a quasi-local conservation law to define what it means to reflect gravitational radiation. We plan to refine this idea in future work.

### 3.5.3 Gauge Controlling BCs

Finally, the operator

$$G_{\mu\nu}{}^{\alpha\beta} \equiv 2\ell_{(\mu}k_{\nu)}k^{(\alpha}\ell^{\beta)} - 2k_{(\mu}\sigma_{\nu)}{}^{(\alpha}\ell^{\beta)} + k_{\mu}k_{\nu}\ell^{\alpha}\ell^{\beta}, \quad (3.48)$$

controls the 4 incoming gauge degrees of freedom. It has a complementary operator

$$G_{\mu\nu}{}^{\alpha} \equiv k_{(\mu}\sigma_{\nu)}{}^{\alpha} + k_{\mu}k_{\nu}\ell^{\alpha} + \ell_{(\mu}k_{\nu)}k^{\alpha}, \quad (3.49)$$

that satisfies  $G_{\mu\nu}{}^{\alpha\beta}G_{\alpha\beta}{}^{\epsilon} = G_{\mu\nu}{}^{\epsilon}$ . One can relate the remaining components of  $U_{\mu\nu}^{-\text{BC}}$  to the incoming derivatives of  $n^{\mu}$ , effectively controlling the incoming derivatives of the lapse and shift

$$\ell^{\sigma}\partial_{\sigma}n^{\beta} = -\left(g^{\beta\nu} + \frac{1}{2}n^{\beta}n^{\nu}\right)n^{\mu}U_{\mu\nu}^{-}. \quad (3.50)$$

Although it was shown in Eqns. (3.11-3.12) that the selection of  $H_{\mu}$  can be thought of as first order evolution equations for the lapse and shift, these equations are *implicit* as they are not directly evolved, and are implied instead by the second order system of GH evolution equations. This means that we are free to choose a set of first order evolution equations for the lapse and shift only on the boundaries, which is what the operator  $G_{\mu\nu}{}^{\alpha\beta}$  specifies. For simplicity we can select a model  $\mathcal{G}_{\alpha\beta}^{\text{BC}}$  and apply it with

$$G_{\mu\nu}{}^{\alpha\beta}U_{\alpha\beta}^{-\text{BC}} = G_{\mu\nu}{}^{\alpha\beta}\mathcal{G}_{\alpha\beta}^{\text{BC}}. \quad (3.51)$$

### 3.5.4 Discussion on BC choices

Together with a user specified set  $\mathcal{C}_\mu^{\text{BC}}$ ,  $h_{\mu\nu}^{\text{BC}}$ , and  $\mathcal{G}_{\mu\nu}^{\text{BC}}$ , we fix all 10 incoming degrees of freedom in the metric, each component of which has a clear interpretation.

A natural choice for the value of the constraints on the boundary is  $\mathcal{C}_\mu^{\text{BC}} = 0$ . One can also inject a model of constraint violating modes for numerical tests and constraint damping verification if desired. Although  $h_{\mu\nu}^{\text{BC}}$  and  $\mathcal{G}_{\mu\nu}^{\text{BC}}$  are left arbitrary, bad choices can be made, such as choices that introduce discontinuities into the metric. The GH equations can develop shocks when discontinuous initial data and BCs are used. The simplest choice that avoids this possibility is  $h_{\mu\nu}^{\text{BC}} = \mathcal{G}_{\mu\nu}^{\text{BC}} = U_{\mu\nu}^{-\text{init}}$ , which is effectively the same BCs used for these components by default in [41]. We will use this choice for simplicity in this work.

It is important to note that the BCs here are applied via first derivatives of the metric, effectively acting as a Dirichlet BC with respect to the evolved state-vector, whereas in [41] BCs are applied via *second* derivatives of the metric, effectively controlling  $\partial_t U_{\mu\nu}^-$  rather than  $U_{\mu\nu}^-$ . The control of  $\partial_t U_{\mu\nu}^-$  allows for the imposition of constraint transparent/absorbing boundaries, where constraint violating modes are allowed to leave the computational domain through the boundaries. In contrast, the BCs used here enforce the *value* of  $\mathcal{C}_\mu$ , which was first shown to be well-posed in [70] and tested numerically in [71], although this BC method is not in common use today. These BCs thus act like a Dirichlet condition on  $\mathcal{C}_\mu$ , allowing constraint violating modes to reflect off of the boundaries of the domain. We consider this behavior acceptable as long as the constraint damping rate is adequate. The reason for this difference is so that the BCs can be implemented using SATs, a weak application of BCs that has been shown to be essential in ensuring SBP properties are obeyed properly [29]. In principle, one could evolve an equation for  $\partial_t \mathcal{C}_\alpha^{\text{BC}}$  alongside the GH evolution equations and still apply the BCs as we do here to impose the same constraint transparent boundaries of [41], but we do not find this necessary. In fact, by imposing  $\mathcal{C}_\alpha^{\text{BC}} = \partial_t \mathcal{C}_\alpha^{\text{BC}} = 0$ , we ensure that in the vicinity of the boundary, the Einstein constraints are satisfied, which is desirable in the strong gravity region of the spacetime where constraint violations and numerical errors are likely to spoil the evolution.

## 3.6 Embedded Boundary SBP Methods

In an effort to use the same modern numerical methods that we have used in our previous work, we consider here a class of embedded boundary SBP methods. This relatively recently introduced class of numerical methods allow for the evolution of systems on arbitrarily shaped domains. The general idea is to use a rectangular grid, and Cartesian-like

coordinates, to evolve the equations in the bulk, where spatial derivatives are calculated using an SBP based finite differencing technique whose stencils terminate wherever they intersect a boundary of the domain.

One such method introduced in [67] allows the boundary position to be between grid points, and the boundary values are obtained and BCs applied using interpolation or extrapolation operators. This method is easy to implement, as nothing more than a rectangular grid of values is needed, with points inside a closed boundary within this bulk grid just “turned off” as they are not evolved. The authors of [67] do outline several complications of this method that require extra care, including special situations where thin domain geometries do not allow for enough grid points to fit a finite differencing stencil.

Another method introduced in [72] instead includes grid values on the boundary itself. For every point where a connecting grid line intersects a boundary, a grid value located there is introduced and evolved. This method is less straightforward to implement, as the points on a boundary do not necessarily fit in the normal rectangular structure of a grid array, and have to be stored separately and communicate with the bulk domain properly. Adding to the complexity, in order for the points on a boundary to be evolved, one also needs to interpolate finite differencing stencils along directions orthogonal to the intersecting stencil line, as there is not necessarily a stencil possible in these directions with the existing rectangular grid values. However, this method avoids many of the complications of thin domain geometries from the previous method.

As far as we are aware, an embedded boundary SBP finite differencing method that has been proven for dimensions more than one does not yet exist. Both of the methods we cite prove SBP for one dimension, then construct a multidimensional approach as if each connecting line in the grid is its own one dimensional problem. This falls short of an SBP proof for multidimensional problems, and [67] adds numerical dissipation to the system to ensure stability. The authors from [72] report to solve nonlinear problems without the use of numerical dissipation however.

In this work, we adopt the method from [67]. The operators from this method are defined in terms of two distance parameters,  $\alpha_l$  and  $\alpha_r$ , that designate where the physical boundary is (in units of the grid spacing) from its closest grid points on the left and right of the stencil respectively, which is visualized in Figure 3.1. These parameters were originally defined to range from  $-0.5 \leq \alpha_{l,r} < 0.5$ , positive (negative) values indicating that the last grid point is just inside (outside) of the boundary relative to the computational domain. This is inconvenient however, as this parameter range allows for trapped points, grid points that cannot be assigned a finite differencing stencil in one or more directions, and thus the value of the derivative must be extrapolated there. This can be avoided

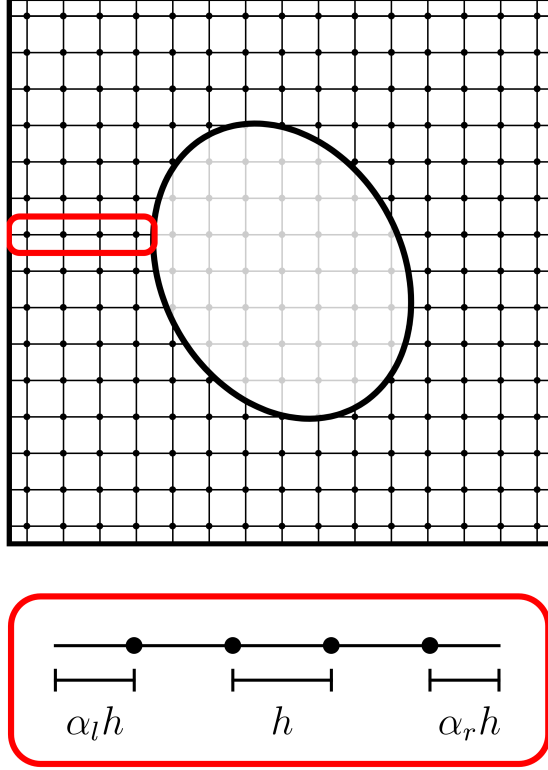


Figure 3.1: Visualization of the embedded boundary method from [67] on a 2D slice, here shown with a square outer boundary and an elliptical inner boundary (bold lines/curves), with the computational grid points shown connected with thin lines. The light grey grid points within the ellipse exist in memory on the bulk grid, but are not evolved. The embedded boundary method considers all of the connecting grid lines and defines finite differencing stencils along these lines that depend on the grid spacing  $h$  as well as the distance parameters  $\alpha_l$  and  $\alpha_r$  that dictate where the boundary of the domain lies relative to the ends of each of the grid lines. The red region zooms in to one such line to visualize these parameters.

completely (specifically for the case of a convex closed boundary with the computational domain surrounding it) if the parameter range is restricted to  $0 \leq \alpha_{l,r} < 1$  instead. For the fourth order and sixth order accurate stencils in [67], the SBP norm is not positive definite for this parameter range, but the second order accurate operators  $D_{2-1}$  are, so for simplicity we will use these operators in this work with this parameter range. This ensures that the boundary is always outside of the computational grid array, and the values on the boundary are always extrapolated rather than interpolated. As is required for SBP operators with diagonal norms, there is reduced accuracy near the boundary points. The operator  $D_{2-1}$  is second order accurate in the interior but only first order accurate near

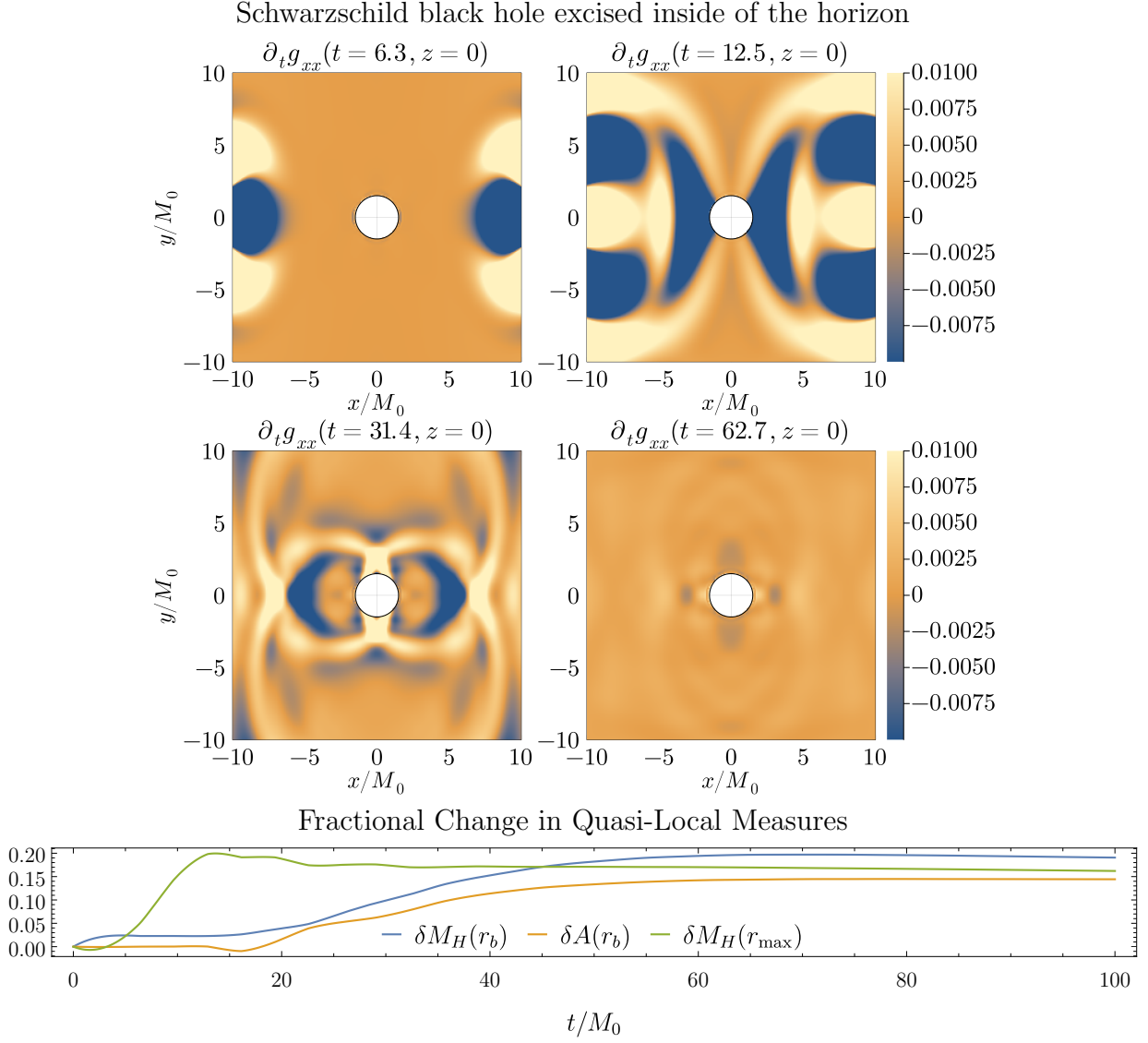


Figure 3.2: Simulation of GW scattering on a Schwarzschild black hole of initial mass  $M_0 = 1$ . The black hole is excised *inside* the horizon at  $r_b = 1.5M_0$ . Top panels show  $\partial_t g_{xx}$  at several times on the  $z = 0$  slice. Bottom panel shows the fractional change in the surface area of the inner boundary  $A(r_b)$  as well as the Hawking mass  $M_H$  evaluated at  $r_b$  and the largest sphere in the cubical domain  $r_{\max}$ .

the boundaries.

From [67], we obtain the SBP derivative operator  $D_{2-1}(\alpha_{l,r})$ , its corresponding norm operator  $\Sigma(\alpha_{l,r})$ , and a set of first order accurate extrapolation operators  $e_{l,r}(\alpha_{l,r})$ . Since

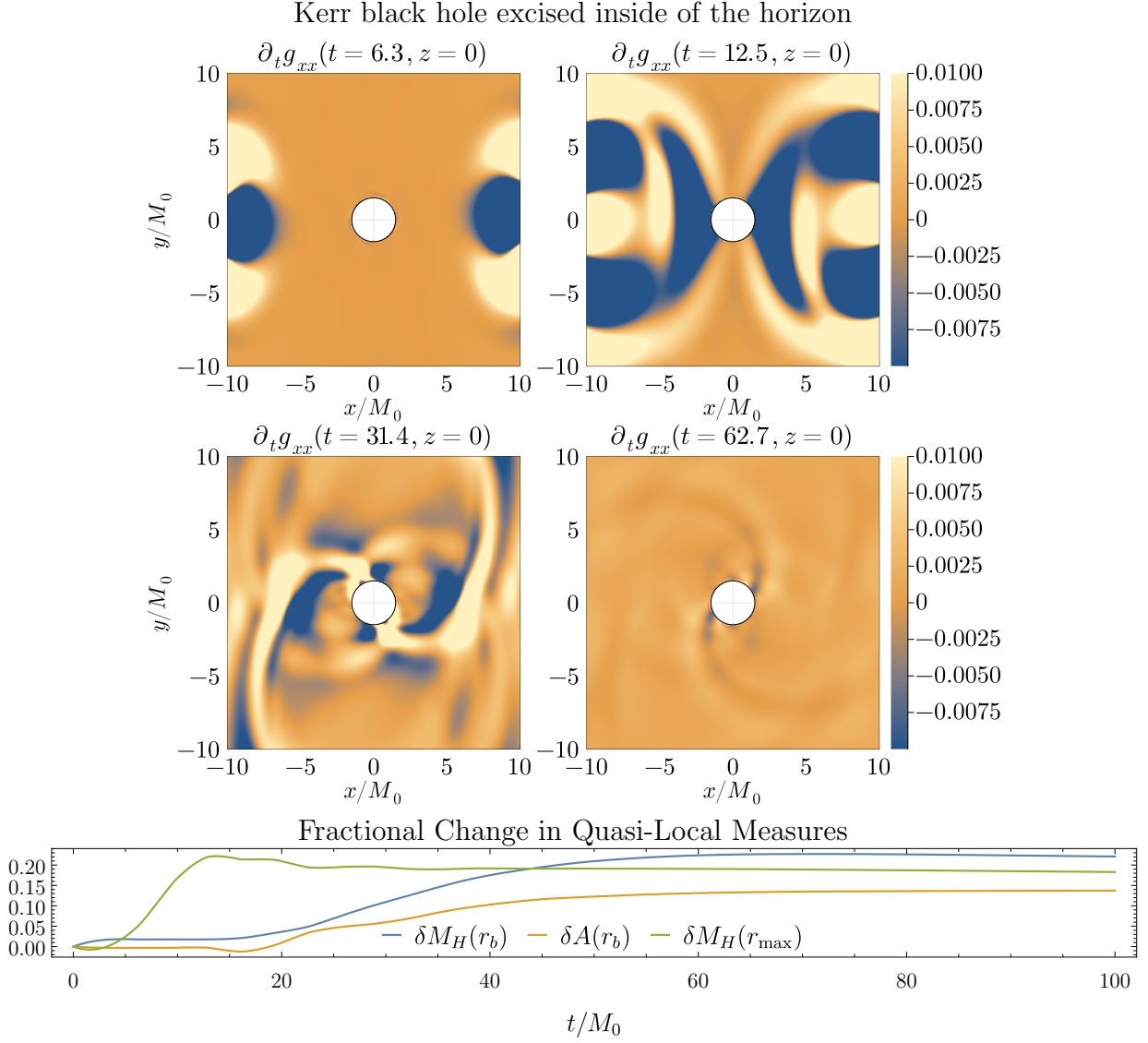


Figure 3.3: Simulation of GW scattering on a Kerr black hole of initial mass  $M_0 = 1$  and spin parameter  $a = 0.5M_0$ . The black hole is excised *inside* the horizon at  $r_b = 1.5M_0$ . Top panels show  $\partial_t g_{xx}$  at several times on the  $z = 0$  slice. Bottom panel shows the fractional change in the surface area of the inner boundary  $A(r_b)$  as well as the Hawking mass  $M_H$  evaluated at  $r_b$  and the largest sphere in the cubical domain  $r_{\max}$ .

the boundary does not necessarily lie on a grid point, the application of BCs needs to be extrapolated. At a boundary intersecting a grid line on its left for example, the SAT

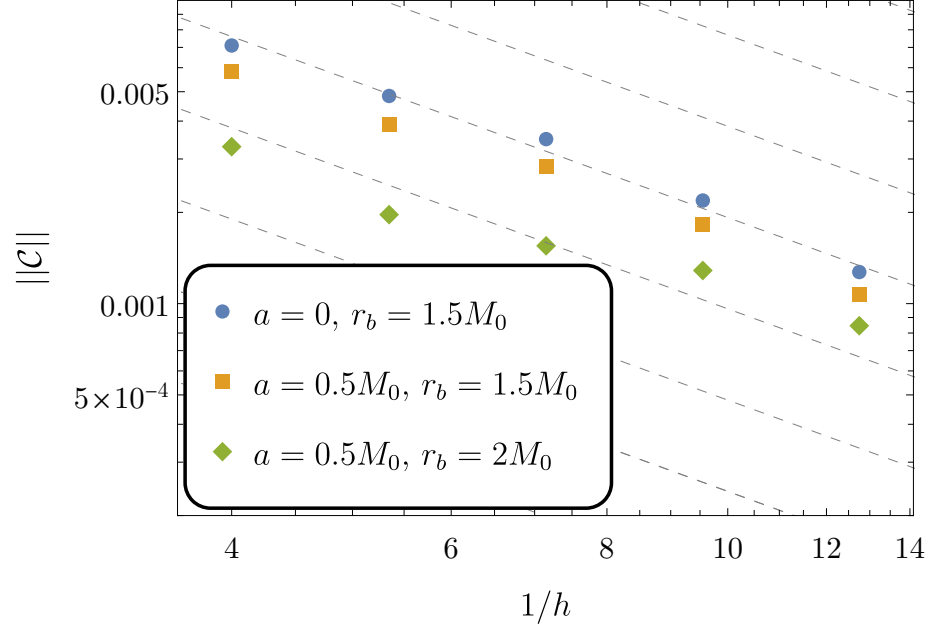


Figure 3.4: Convergence of the constraint norm evaluated at  $t = 100M_0$  as the resolution is increased for the various simulations presented. Dashed lines are  $\propto h^{1.5}$  to make it apparent that since the operators we use are second order accurate in the interior and first order at the boundaries, a global convergence rate of about 1.5 is achieved.

application of BCs is

$$\partial_t P_{\mu\nu} = \dots - c_- \Sigma^{-1} e_l [P_{\mu\nu}^{\text{BC}} - e_l P_{\mu\nu}] , \quad (3.52)$$

$$\partial_t d_{i\mu\nu} = \dots - c_- \Sigma^{-1} e_l [d_{i\mu\nu}^{\text{BC}} - e_l d_{i\mu\nu}] . \quad (3.53)$$

This is very similar to adding an exponential decay term to the evolution equations at the boundary (as is the general idea of SAT techniques), except that the value of the state vector at the boundary is extrapolated, and the exponential decay term is applied at the boundary point using an extrapolation operator as well. The decay rate is set to the incoming coordinate speed  $c_-$  as we showed is necessary in [44], and thus the BCs are applied more weakly the closer the boundary worldtube is to a null hypersurface where  $c_- \rightarrow 0$ .

### 3.7 Results

Here, we demonstrate several 3D simulations to showcase our altered formulation, our new BC framework, and the embedded boundary numerical method. We study the evolution of GW scattering on spinning and non-spinning black holes and cases where the center of the hole is excised just inside or just outside of the apparent horizon.

In the following set of simulations presented, we keep as many things the same as possible to aid in direct comparison. We use initial mass  $M_0 = 1$  for the black holes and constraint damping parameters  $\gamma_0 = \gamma_2 = 1/M_0$ . We also add numerical dissipation to aid in the stability of the simulation. This is done as

$$\partial_t \vec{U} = \dots + \varepsilon D_4 \vec{U}, \quad (3.54)$$

where  $\varepsilon$  is the amount of dissipation and the dissipation operator  $D_4$  that pairs with the second order finite differencing operators we use in this work is found in [67]. We use  $\varepsilon = 0.1$  in all of the simulations presented here.

We track several quasi-local measures of mass and surface area (for numerical calculation details of closed surface integrals, see Appendix C). The surface area of the inner boundary is tracked because although the boundary is fixed in coordinate space, it may still physically grow/shrink. The black hole may also move into the computational domain if it is given linear momentum, but we inject GWs from two opposite sides at once to ensure this does not occur. The surface area of a coordinate sphere is defined as

$$A(r) = \oint_{S(r)} dS(r), \quad (3.55)$$

where  $S(r)$  is a coordinate sphere of radius  $r$  and  $dS(r)$  is the surface area element on that sphere. To measure the accretion of mass on the hole, we use the Hawking mass as a measure of the mass contained in a coordinate sphere

$$M_H(r) = \sqrt{\frac{A(r)}{16\pi}} \left( 1 + \frac{1}{16\pi} \oint_{S(r)} \rho \rho' dS(r) \right), \quad (3.56)$$

where  $\rho$  and  $\rho'$  are the expansions of ingoing and outgoing null geodesics at the sphere, respectively. The integrand of the closed surface integral in this definition can also be expressed as [23]

$$\rho \rho' = (\sigma^{\mu\nu} K_{\mu\nu})^2 - (\bar{\nabla}^i s_i)^2. \quad (3.57)$$

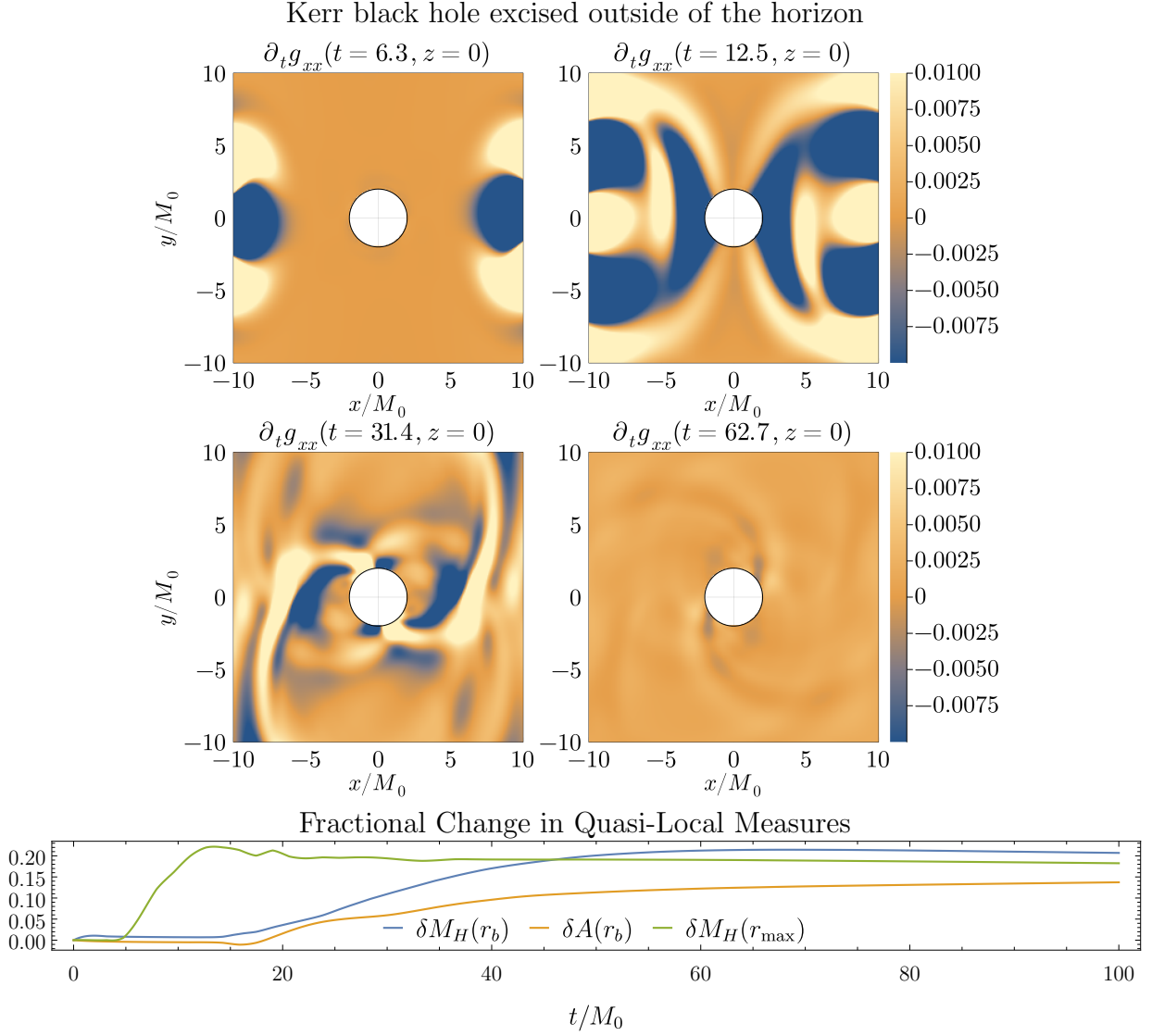


Figure 3.5: Simulation of GW scattering on a Kerr black hole of initial mass  $M_0 = 1$  and spin parameter  $a = 0.5M_0$ . The black hole is excised *outside* the horizon at  $r_b = 2M_0$ , since the outer horizon is initially at  $r_+ \approx 1.87M_0$ . Top panels show  $\partial_t g_{xx}$  at several times on the  $z = 0$  slice. Bottom panel shows the fractional change in the surface area of the inner boundary  $A(r_b)$  as well as the Hawking mass  $M_H$  evaluated at  $r_b$  and the largest sphere in the cubical domain  $r_{\max}$ . With the GW BCs we apply at the inner boundary (i.e. keeping these components constant), we see largely the same behavior from the quasi-local measures as the simulations excised inside the horizon, suggesting that these BCs lead to the absorption/transmission of GWs.

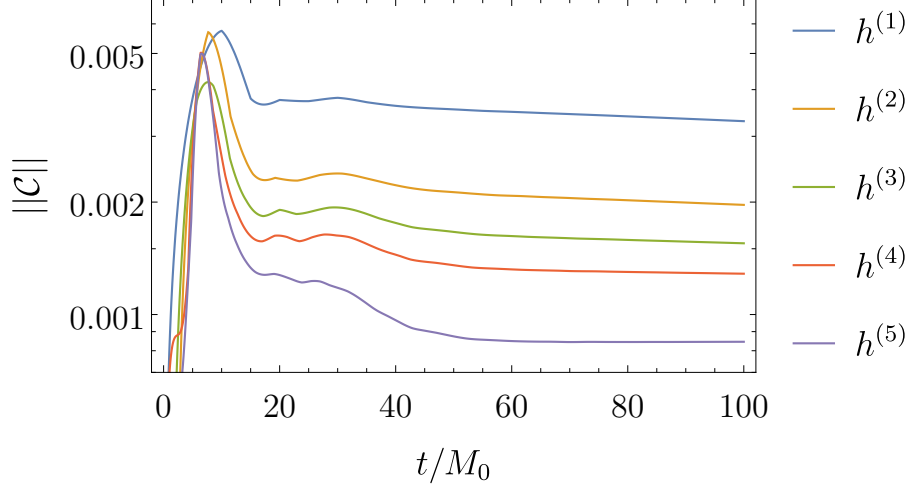


Figure 3.6: Behavior of the gauge constraint norm over time for the five resolutions ( $h^{(i)}$ ) in the Kerr black hole case with the boundary just outside the spinning black hole ( $a = 0.5M_0$  and  $r_b = 2M_0$ ). We see that even though constraint violations are introduced when GWs are injected, they are damped out and settle to a finite value, which converges to zero with increased resolution. The other two simulations exhibit identical behavior in this respect.

We also define the gauge constraint norm as

$$\|\mathcal{C}\|^2 = \frac{\int m^{\mu\nu} \mathcal{C}_\mu \mathcal{C}_\nu dV}{\int dV}, \quad (3.58)$$

to track the convergence and damping of the constraint violating modes.

We present five different resolutions where  $h^{(i)} = 3h^{(i-1)}/4$  as the resolution is increased by a factor of  $4/3$  from one to the next starting at  $h^{(1)} = 0.25M_0$ . The computational domain consists of a cube of volume  $(20M_0)^3$  with an inner excised sphere of various radii, and we only consider grid spacings that are the same in all three coordinate directions. We use a third order accurate Runge-Kutta algorithm to advance the equations with a time step  $h_t = h/5$ , which reflects the worst case CFL factor estimates from [67].

### 3.7.1 Schwarzschild GW Scattering

Here, we consider the initial condition of a Schwarzschild black hole in Kerr-Schild coordinates. This completely defines the metric  $g_{\mu\nu}^{\text{init}}$  on the initial slice and the gauge functions  $H_\mu = \Gamma_\mu^{\text{init}}$  we use for all time. Then we use our initial condition formalism to ensure

$\mathcal{C}_\mu^{\text{init}} = \mathcal{C}_{i\mu\nu}^{\text{init}} = 0$ . The remaining components of  $P_{\mu\nu}$  are set by requiring  $\partial_t g_{\mu\nu}^{\text{init}} = 0$ . We then inject GWs using the following model:

$$f_{\text{GW}}(x^\alpha) = A_{\text{GW}}[r_e(x^\alpha) + 1]^4[r_e(x^\alpha) - 1]^4, \quad (3.59)$$

defined in a region  $r_e < 1$  and is zero if  $r_e \geq 1$  where

$$r_e^2(x^\alpha) = [(x - x_0 + v_x t)/r_x]^2 + (y/r_y)^2 + (z/r_z)^2. \quad (3.60)$$

This defines an ellipsoidal region with semi-axes  $r_i$  that moves at  $x$ -directed velocity  $v_x$  from its initial  $x$ -position (outside the computational domain)  $x_0$ . The amplitude  $A_{\text{GW}}$  can then be tuned to add a desired amount of mass in GWs. We use  $A_{\text{GW}} = 130$ , which results in an increase in Hawking mass of the hole by about 20%. The polynomial in Eq. (3.59) ensures that the first three derivatives are continuous while allowing  $f_{\text{GW}}$  to be exactly zero where  $r_e \geq 1$ . We inject this model in the following fashion

$$P_{\mu\nu}{}^{\alpha\beta} U_{\alpha\beta}^{-\text{BC}} = P_{\mu\nu}{}^{\alpha\beta} U_{\mu\nu}^{-\text{init}}(1 + f_{\text{GW}}). \quad (3.61)$$

In this and following simulations, we use  $r_y = r_z = 10M_0$ ,  $r_x = 5M_0$ ,  $v_x = \pm 1$ , and  $x_0 = (20 \pm 5)M_0$  for injections from the  $\mp x$ -directions. We then evolve the spacetime until the metric and quasi-local measures settle to approximately constant final values at  $t = 100M_0$ . Results are depicted in Figure (3.2). We track the fractional change  $[\delta f(t) \equiv (f(t) - f(0))/f(0)]$  in both the Hawking mass of the inner sphere  $M_H(r_b)$  as well as its value at the largest sphere in the domain  $M_H(r_{\text{max}})$ . We also track the surface area of the inner sphere  $A(r_b)$ . As should be expected,  $M_H(r_{\text{max}})$  increases first, followed by  $M_H(r_b)$ , until they settle close to the same value at late time. The surface area  $A(r_b)$  increases as well.

### 3.7.2 Kerr GW Scattering

In the same setup as the previous section, we use now a spinning black hole. We use a metric expressed in so-called Spherical Kerr-Schild coordinates defined in [73], (see Appendix D). This set of coordinates is transformed relative to traditional Kerr-Schild coordinates such that the horizons are spherical in coordinate space (as opposed to oblate ellipsoids). This allows us to place a spherical boundary at a constant coordinate distance from the horizon as we did in the previous section. We use spin  $a = 0.5M_0$  and the same inner boundary  $r_b = 1.5M_0$  which is still inside the outer horizon of the hole at  $r_+ \approx 1.87M_0$ . We inject GWs in the same fashion as the Schwarzschild black hole and evolve the system until the

metric and quasi-local measures settle to approximately constant final values at  $t = 100M_0$ , with results depicted in Figure (3.3). This simulation exhibits largely the same behavior in quasi-local measures as the Schwarzschild case, except both  $M_H(r_b)$  and  $M_H(r_{\max})$  seem to increase slightly more by  $t = 100M_0$ .

Next we showcase the same simulation, but instead with  $r_b = 2M_0$ , just *outside* of the outer horizon. The results are depicted in Figure (3.5). When the hole is excised inside the horizon,  $M_H(r_b)$  increases by 22%, but when it is excised outside the horizon,  $M_H(r_b)$  increases by 20%, suggesting that the GW BC choice at the inner boundary,  $h_{\mu\nu}^{\text{BC}} = U_{\mu\nu}^{-\text{init}}$ , is a mostly transmitting/absorbing condition, with a reflection of about 10% of the incident waves' mass (at least for this specific setup). The set of simulations we present are meant to showcase the stability we are able to achieve with the formalism and numerical methods we use when a boundary is placed in the strong gravity region of a dynamical spacetime, which has been notoriously difficult to achieve numerically in the past.

The convergence of the constraint norm for all three simulations is depicted in Figure (3.4), where the  $D_{2-1}$  operator achieves less than second order convergence as is expected with SBP operators of this type. The behavior of the constraint norm over the period of the last simulation is depicted in Figure (3.6). The constraints increase as GWs are injected, but they soon damp out as expected, with increased resolution converging to zero at the final time.

## 3.8 Future Work

The numerical methods we demonstrate in this work allow for much more complex IBVPs that we plan to study further, including

- Non-spherically shaped and non-convex inner boundaries
- Dynamical inner boundaries
- Non-cubical outer boundaries
- Higher accuracy operators

In particular, successful evolution of a dynamical boundary would allow for a much simplified binary black hole excision setup with finite differencing algorithms. This requires a way to initialize grid points that enter the computational domain as the boundary moves

across the grid, which is usually done with extrapolation techniques. Once binary systems can be demonstrated, the addition of Cauchy characteristic matching would allow for the extraction of gravitational waveforms at infinity while preserving computational efficiency. Whether the boundary is placed inside or outside of an apparent horizon, its shape and movement over time should be dictated by an evolution formalism that ties the boundary to the black holes. We plan to study further how such an evolution can be achieved numerically when coupled with these embedded boundary methods.

We proposed in this work to use quasi-local conservation laws to define what it means to reflect gravitational radiation, as well as how to interpret what a given set of BCs implies about the mass, linear momentum, and angular momentum within a closed boundary as the system evolves over time. We plan to refine this concept into a proper mathematical framework that one could use to derive BCs for a desired boundary behavior.

### 3.9 Conclusion

We have demonstrated successful black hole excision simulations both inside and outside of an apparent horizon on a strictly rectangular grid for the first time, which is the debut of embedded boundary finite differencing methods to the numerical relativity community. We have also shown that we can run stable numerical relativity simulations in a relatively small domain. This is important for Cauchy characteristic matching techniques, where the Cauchy evolution domain can in principle be made small, close to the scale of merging black holes, for example, to dramatically save on computational cost while retaining numerical stability and accurate gravitational waveforms at infinity. We presented a boundary condition framework based on controlling first derivatives of the metric in the generalized harmonic formulation, which has allowed us to cast Einstein's equations as an SBP-SAT scheme. This framework can be applied to other numerical methods common in the field, such as spectral methods, to obtain simulations that are numerically stable even when the computational domain has boundaries in the strong gravity regime. This marks a big leap toward our ultimate goal to evolve binary black hole simulations with boundary surfaces drawn just outside of the apparent horizons of the holes. This will allow us to impose quantum gravity motivated behavior on these boundary surfaces to obtain the first gravitational waveforms of black hole echoes from numerical relativity.

# Chapter 4

## Boundary Conditions Based On Quasi-local Conservation Laws

### Preface

This chapter contains a novel formalism for applying boundary conditions on the radiative degrees of freedom in general relativity based on controlling the flux in quasi-local conservation laws. Section 4.1 introduces local and quasi-local conservation laws. Section 4.2 considers electromagnetic waves as an analogous system to gravitational waves in the sense that it contains two polarization modes. Finally, Section 4.3 considers quasi-local energy conservation as a way to define what it means to reflect gravitational waves.

This work has not been previously published, but is planned to be expanded on and published in the future. References to ‘we’ in this chapter refer to the author of this thesis and the reader.

## 4.1 Introduction

Now that the formulation, numerical methods, and boundary framework have been implemented and numerically tested in Chapters 2 and 3 with and without symmetry assumptions, we can work to derive boundary conditions on gravitational waves. Although there is no local definition of gravitational wave properties, like energy, linear momentum, and angular momentum, there are quasi-local definitions of these concepts. Quasi-local conservation laws are introduced and carefully studied in [65, 74], and this chapter will introduce many concepts covered in these works and then derive boundary conditions based on controlling the flux of quasi-local energy.

Locally measured and conserved quantities have local conservation laws, where a conservation law is called local if it relates the change in a quantity that is the result of an integral over a 3-space, to the flux of this quantity through a 2-surface. To see an example of this, we consider an arbitrary stress energy tensor  $T^{\mu\nu}$  and a vector field  $\xi^\mu$  residing in the  $3+1$  manifold  $\mathcal{M}$ . Due to the properties of the covariant derivative, the following always holds:

$$\nabla_\mu(T^{\mu\nu}\xi_\nu) = (\nabla_\mu T^{\mu\nu})\xi_\nu + T^{\mu\nu}\nabla_{(\mu}\xi_{\nu)}. \quad (4.1)$$

On the right hand side, the first term vanishes because  $\nabla_\mu T^{\mu\nu} = 0$  is a fundamental property of the stress energy tensor. The second term does not vanish unless  $\xi^\mu$  is a Killing vector. If we consider a time independent spacetime that contains a timelike Killing vector  $\xi_{(t)}^\mu = \partial_t x^\mu$ , then with respect to this vector field, the left hand side vanishes and we have a locally conserved current.

$$\nabla^\mu(T_{\mu\nu}\xi_{(t)}^\nu) \equiv \nabla^\mu J_\mu = 0. \quad (4.2)$$

The Gauss divergence theorem states that the divergence of a vector field integrated over the manifold  $\mathcal{M}$  is related to a closed hypersurface integral over all of the hypersurfaces bounding  $\mathcal{M}$ :

$$\int \nabla^\mu J_\mu d\mathcal{M} = \oint m^\mu J_\mu d(\partial\mathcal{M}). \quad (4.3)$$

The left hand side represents an integral over  $\mathcal{M}$  and the right hand side represents an integral over all of the hypersurfaces that bound  $\mathcal{M}$ , denoted  $\partial\mathcal{M}$ , that have outward pointing unit normal  $m^\mu$ . Since  $J^\mu$  is a conserved current, the left hand side vanishes, leaving

$$\oint m^\mu J_\mu d(\partial\mathcal{M}) = 0. \quad (4.4)$$

We consider  $\mathcal{M}$  bounded by initial and final spatial hypersurfaces  $\mathcal{N}_i$  and  $\mathcal{N}_f$  respectively, and a timelike worldtube  $\mathcal{B}$ , shown in Figure 4.1. The integral in Eq. (4.4) then splits into three pieces, one for each of  $\mathcal{N}_i$ ,  $\mathcal{N}_f$ , and  $\mathcal{B}$ . We can identify  $m^\mu \rightarrow n^\mu$  and  $m^\mu \rightarrow r^\mu$  for the two hypersurfaces  $\mathcal{N}_f$  and  $\mathcal{B}$  respectively, but  $m^\mu \rightarrow -n^\mu$  for  $\mathcal{N}_i$  as by convention  $n^\mu$  points into the future. The hypersurface volume element is taken as negative for spacelike hypersurfaces and positive for timelike ones. We have then

$$-\int n^\mu J_\mu d\mathcal{N}_f + \int n^\mu J_\mu d\mathcal{N}_i + \int r^\mu J_\mu d\mathcal{B} = 0. \quad (4.5)$$

Now we take the limit where  $\mathcal{N}_i$  approaches  $\mathcal{N}_t$  from below and  $\mathcal{N}_f$  approaches  $\mathcal{N}_t$  from above in order to write an instantaneous conservation law. The volume element of the worldtube is related to an instantaneous surface area element by the lapse  $d\mathcal{B} = \alpha dS$ . We then use the fundamental theorem of calculus to write

$$\partial_t \int n^\mu J_\mu dV = \oint \alpha r^\mu J_\mu dS, \quad (4.6)$$

where  $dV$  is the volume element on  $\mathcal{N}_t$ . We can see that this is indeed a local conservation law, as it relates the change in a 3-volume integral to the flux through a closed 2-surface. Unfortunately, this can only be written as such when a spacetime has a Killing symmetry, which will not be the case for physically realistic gravitational wave sources.

Instead, in order to write a conservation law without symmetry assumptions, we start one dimension lower, within only the worldtube  $\mathcal{B}$ . For any tensor field  $T_{\mathcal{B}}^{\mu\nu}$  and vector field  $\psi^\mu$  within  $\mathcal{B}$ , we have

$$\hat{\nabla}_\mu (T_{\mathcal{B}}^{\mu\nu} \psi_\nu) = (\hat{\nabla}_\mu T_{\mathcal{B}}^{\mu\nu}) \psi_\nu + T_{\mathcal{B}}^{\mu\nu} \hat{\nabla}_{(\mu} \psi_{\nu)}, \quad (4.7)$$

where  $\hat{\nabla}_\mu$  is the covariant derivative with respect to the metric on  $\mathcal{B}$ ,  $h_{\mu\nu}$ . The current  $J^\mu = T_{\mathcal{B}}^{\mu\nu} \psi_\nu$  now lies tangent to  $\mathcal{B}$ . Gauss' theorem in this context is instead split into two pieces, initial and final bounding 2-surfaces  $S_i$  and  $S_f$  respectively:

$$\int \hat{\nabla}^\mu J_\mu d\mathcal{B} = \oint m^\mu J_\mu d(\partial\mathcal{B}) = -\oint n_S^\mu J_\mu dS_f + \oint n_S^\mu J_\mu dS_i, \quad (4.8)$$

where  $n_S^\mu$  is a normalized projection of  $n^\mu$  onto the worldtube. Integrating Eq. (4.7) over  $\mathcal{B}$  and applying Gauss' divergence theorem, we obtain

$$-\oint n_S^\mu J_\mu dS_f + \oint n_S^\mu J_\mu dS_i = \int [(\hat{\nabla}_\mu T_{\mathcal{B}}^{\mu\nu}) \psi_\nu + T_{\mathcal{B}}^{\mu\nu} \hat{\nabla}_{(\mu} \psi_{\nu)}] d\mathcal{B}. \quad (4.9)$$

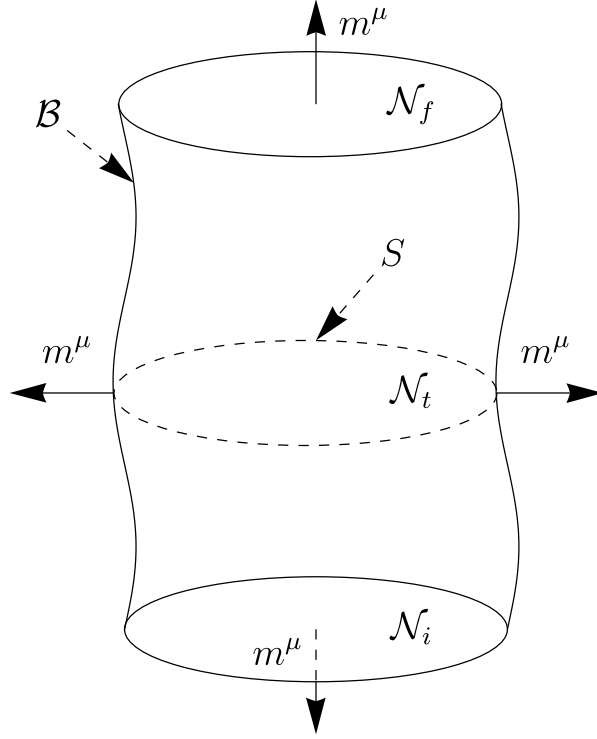


Figure 4.1: Diagram labeling the bounding hypersurfaces in Gauss' divergence theorem, where time runs on the vertical, the 3-space is horizontal, and null rays run along  $45^\circ$  lines. The bounding hypersurfaces to the  $3+1$  manifold  $\mathcal{M}$  are split into an initial spacelike hypersurface  $\mathcal{N}_i$ , a final spacelike hypersurface  $\mathcal{N}_f$ , and a timelike enclosing worldtube  $\mathcal{B}$ . The vector field  $m^\mu$  is always orthogonal and outward pointing to the bounding hypersurfaces, regardless of if it is timelike or spacelike.

Again taking the limit as  $S_i$  approaches  $S_t$  from below and  $S_f$  approaches  $S_t$  from above, we obtain an instantaneous quasi-local conservation law

$$\partial_t \oint n_\mu^S T_{\mathcal{B}}^{\mu\nu} \psi_\nu dS = - \oint \alpha [(\hat{\nabla}_\mu T_{\mathcal{B}}^{\mu\nu}) \psi_\nu + T_{\mathcal{B}}^{\mu\nu} \hat{\nabla}_{(\mu} \psi_{\nu)}] dS. \quad (4.10)$$

This conservation law is called quasi-local, as it relates the change in a 2-surface integral to the flux through a 2-surface, and thus only relates to dynamics in the vicinity of  $S$ . This relation holds for any tensor field  $T_{\mathcal{B}}^{\mu\nu}$  and vector field  $\psi_\mu$  in the worldtube  $\mathcal{B}$ . However, we consider choosing  $T_{\mathcal{B}}^{\mu\nu}$  to be the Brown-York stress tensor [75], which is defined as

$$T_{\mathcal{B}}^{\mu\nu} = -\frac{1}{8\pi}(\kappa_{\mu\nu} - h_{\mu\nu}\kappa), \quad (4.11)$$

where  $\kappa_{\mu\nu} = h_\mu^\alpha h_\nu^\beta \nabla_\alpha r_\beta$  is the extrinsic curvature of  $\mathcal{B}$ . This allows us to relate its divergence in  $\mathcal{B}$  to the projection of the 4 dimensional stress energy tensor via the Gauss-Codazzi identity and the Einstein field equations:

$$\hat{\nabla}_\mu T_{\mathcal{B}}^{\mu\alpha} = -\frac{1}{8\pi} h^\alpha{}_\mu r_\nu T^{\mu\nu}. \quad (4.12)$$

This allows us to write a family of instantaneous quasi-local conservation laws

$$\partial_t \oint n_\mu^S T_{\mathcal{B}}^{\mu\nu} \psi_\nu dS = \oint \alpha \left[ \frac{1}{8\pi} T^{\mu\nu} r_\mu \psi_\nu - T_{\mathcal{B}}^{\mu\nu} \hat{\nabla}_{(\mu} \psi_{\nu)} \right] dS, \quad (4.13)$$

for any vector field  $\psi^\mu$  tangent to  $\mathcal{B}$ . The 2-surface flux on the right hand side depends on two terms, one that comes purely from the matter content in the spacetime flowing through the 2-surface, and another term that is purely geometrical and contains information regarding the gravitational waves flowing through the surface as well as the dynamics of the 2-surface itself.

Choosing the vector field  $\psi^\mu$  affects the interpretation of what kind of quasi-local conservation law is being represented. Choosing a timelike  $\psi^\mu$  invites an interpretation of quasi-local energy conservation, while choosing a spacelike  $\psi^\mu$  invites an interpretation of quasi-local momentum conservation, be it linear or angular. We will focus on timelike choices of  $\psi^\mu$  later in this chapter.

## 4.2 Maxwell's Electrodynamics

As an example of the boundary conditions placed on systems with polarization, we will consider solving the Maxwell equations numerically given a class of boundary conditions. Electromagnetic waves, just like gravitational waves, have two radiative degrees of freedom corresponding to two polarization modes, so this system will be instructive to how boundary conditions can be applied to such systems.

The sourceless Maxwell equations can be expressed in terms of the 4-potential  $A_\mu$  with the Faraday tensor  $F_{\mu\nu} = 2\nabla_{[\mu} A_{\nu]}$ :

$$\nabla^\mu F_{\mu\nu} = 0. \quad (4.14)$$

This system does not have the form of a set of wave equations until we enforce a generalized Lorentz gauge

$$\nabla^\mu A_\mu = H(x^\alpha), \quad (4.15)$$

for any function of spacetime  $H(x^\mu)$ . The equations of motion for  $A^\mu$  then become a set of sourced wave equations [76]

$$\nabla^\mu \nabla_\mu A_\nu = \nabla_\nu H + R_{\mu\nu} A^\mu. \quad (4.16)$$

This system is directly analogous to the generalized harmonic equations in the sense that using  $H(x^\mu)$  to fix the gauge freedom in the bulk has reduced the system to a set of wave-like equations.

If we consider the electromagnetic field as a “test” field, so that it does not couple to spacetime, and we consider its dynamics on a background vacuum spacetime, we can neglect the Ricci tensor term. We then define the auxiliary variables  $\Pi_\nu \equiv -n^\mu \partial_\mu A_\nu$  and  $\psi_{i\nu} \equiv \partial_i A_\nu$ , so that we can write a first order evolution system:

$$\partial_t A_\mu = \beta^i \psi_{i\mu} - \alpha \Pi_\mu, \quad (4.17)$$

$$\partial_t \psi_{i\mu} + \partial_i (\alpha \Pi_\mu - \beta^j \psi_{j\mu}) = 0, \quad (4.18)$$

$$\partial_t \Pi_\mu + \bar{\nabla}_i (\alpha \psi^i_\mu - \beta^i \Pi_\mu) = \alpha \partial_\mu H. \quad (4.19)$$

This system is remarkably similar to the generalized harmonic first order system in the previous chapter. Here, Eq. (4.17) is just the definition of  $\Pi$ , Eq. (4.18) enforces the commutativity of temporal and spatial derivatives, and Eq. 4.19 enforces the Maxwell equations. An analysis of the characteristic matrices yields the characteristic modes:

$$U_\mu^+ \equiv k^\alpha \partial_\alpha A_\mu = -\frac{1}{\sqrt{2}} (\Pi_\mu + s^i \psi_{i\mu}), \quad (4.20)$$

$$U_\mu^- \equiv \ell^\alpha \partial_\alpha A_\mu = -\frac{1}{\sqrt{2}} (\Pi_\mu - s^i \psi_{i\mu}), \quad (4.21)$$

$$U_{\alpha\mu}^\perp \equiv \sigma_\alpha^\beta \partial_\beta A_\mu = \sigma_\alpha^i \psi_{i\mu}. \quad (4.22)$$

The characteristic modes  $U_\mu^\pm$  propagate along the lightcone with characteristic speed  $c_\pm = \pm\alpha - s_i \beta^i$  and  $U_\mu^\perp$  propagates along  $n^\mu$  with characteristic speed  $c_\perp = -s_i \beta^i$ . This system is symmetric hyperbolic, requires no gauge fixing, and has purely causal characteristic speeds, fitting all three of the requirements we set as a starting point for a stable initial boundary value problem.

### 4.2.1 Non-radiative Boundary Conditions

By introducing the generalized Lorentz gauge, we introduce the gauge constraint  $\mathcal{C}$ :

$$\mathcal{C} \equiv \nabla^\mu A_\mu - H(x^\alpha). \quad (4.23)$$

The Maxwell equations imply the evolution of this constraint is a wave equation

$$\nabla^\mu \nabla_\mu \mathcal{C} = 0, \quad (4.24)$$

which ensures that  $\mathcal{C}$  vanishes for all time assuming initial conditions and boundary conditions where  $\mathcal{C} = \partial_t \mathcal{C} = 0$ . Expanding Eq. (4.23) in terms of the characteristic modes leads to a boundary condition on one of the components of  $U_\mu^-$ :

$$k^\mu U_\mu^- = \sigma^{\mu\nu} U_{\mu\nu}^\perp - \ell^\mu U_\mu^+ - \Gamma^\mu A_\mu - H - \mathcal{C}^{\text{BC}}, \quad (4.25)$$

which allows us to control the value of the gauge constraint at the boundary, the natural choice being  $\mathcal{C}^{\text{BC}} = \partial_t \mathcal{C}^{\text{BC}} = 0$ . This fixes one component of the four incoming degrees of freedom in  $U_\mu^-$ , indicating that we have three left to choose.

The Faraday tensor is split into electric ( $E_\mu$ ) and magnetic ( $B_\mu$ ) fields, by picking a set of observers with timelike four velocity  $u_\mu$  to measure them with respect to, where  $u_\mu E^\mu = u_\mu B^\mu = 0$ . In this case, we will consider observers flowing along  $n_\mu$  for simplicity. The Faraday tensor is then given by

$$F_{\mu\nu} = 2n_{[\mu} E_{\nu]} - \varepsilon_{\mu\nu\alpha\beta} n^\alpha B^\beta, \quad (4.26)$$

where  $\varepsilon_{\alpha\beta\mu\nu}$  is the Levi-Civita tensor. The electric field is given by

$$E_\mu = F_{\mu\nu} n^\nu. \quad (4.27)$$

Contracting the electric field with  $s^\mu$  and expressing in terms of the characteristic modes reveals that another component of  $U_\mu^-$  can be set by directly affecting the value of the normal component of the electric field:

$$\ell^\mu U_\mu^- = k^\mu U_\mu^+ + (s^\mu E_\mu)^{\text{BC}}. \quad (4.28)$$

for any desired value  $(s^\mu E_\mu)^{\text{BC}}$  at a point on the boundary. The normal component of the electric field carries information about the Coulomb sources enclosed in the boundary region. If we demand conservation of charge, the monopole moment of  $(s^\mu E_\mu)^{\text{BC}}$  must be constant. Having time varying higher moments of  $(s^\mu E_\mu)^{\text{BC}}$  implies the production of electromagnetic waves from accelerating sources within the closed boundary region. This implies that if we demand that there are no sources within the a closed boundary region for all time, then we can make the simple choice  $(s^\mu E_\mu)^{\text{BC}} = 0$  for the purposes of studying just the radiating degrees of freedom in a computational domain outside of a closed boundary. We now have conditions on both components  $k^\nu U_\nu^-$  and  $\ell^\nu U_\nu^-$ , with the only remaining components being the two tangential ones  $\sigma_\mu{}^\nu U_\nu^-$ .

### 4.2.2 Radiative Boundary Conditions

To write down a conservation law for electromagnetism, we assume the spacetime is independent of time. This grants a Killing vector  $\xi_{(t)}^\mu = \partial_t x^\mu$ , and we can write an energy conservation law:

$$\partial_t \int \xi_{(t)}^\mu n^\nu T_{\mu\nu} d\mathcal{N}_t = \oint \alpha \xi_{(t)}^\mu s^\nu T_{\mu\nu} dS. \quad (4.29)$$

The stress energy tensor in electromagnetism is given by a traceless contraction of the Faraday tensor:

$$T_{\mu\nu} = g^{\alpha\beta} F_{\mu\alpha} F_{\nu\beta} - \frac{1}{4} g_{\mu\nu} F^{\alpha\beta} F_{\alpha\beta}, \quad (4.30)$$

or in terms of the electric and magnetic fields

$$T_{\mu\nu} = \frac{1}{2} (E^2 + B^2) (n_\mu n_\nu + \gamma_{\mu\nu}) - 2n_{(\mu} \varepsilon_{\nu)\lambda\alpha\beta} n^\lambda E^\alpha B^\beta - E_\mu E_\nu - B_\mu B_\nu, \quad (4.31)$$

where  $E^2 = E^\mu E_\mu$ . If we assume Gaussian normal coordinates where  $\alpha = 1$  and  $\beta^i = 0$ , the energy density takes the usual form in terms of the magnitudes of electric and magnetic fields

$$\xi_{(t)}^\mu n^\nu T_{\mu\nu} = \frac{1}{2} (E^2 + B^2), \quad (4.32)$$

while the flux of this energy, called the Poynting flux, is

$$\xi_{(t)}^\mu s^\nu T_{\mu\nu} = \varepsilon_{\mu\nu\alpha\beta} n^\mu s^\nu E^\alpha B^\beta. \quad (4.33)$$

If we install two orthonormal basis vectors  $p_\mu$  and  $q_\mu$  both orthogonal to  $n^\mu$  and  $s^\mu$ , then the 2-metric is given by  $\sigma^{\mu\nu} = p^\mu p^\nu + q^\mu q^\nu$ . We also introduce  $\tilde{\sigma}_{\mu\nu} = \varepsilon_{\alpha\beta\epsilon\mu} n^\alpha s^\beta \sigma^\epsilon_\nu = 2p_{[\mu} q_{\nu]}$ , which is an antisymmetric combination of the basis vectors spanning  $\sigma_{\mu\nu}$ . Controlling the value of the Poynting flux requires a boundary condition of the form

$$\tilde{\sigma}^{\mu\nu} E_\mu B_\nu = F(x^\alpha), \quad (4.34)$$

for some specified flux  $F(x^\alpha)$ , which will allow for the control of the energy flux of electromagnetic waves. We interpret  $F(x^\mu) = 0$  as a perfectly reflecting condition. This is a condition quadratic in the two components of the incoming characteristic modes tangential to the boundary:

$$\begin{aligned} \tilde{\sigma}^{\mu\nu} E_\mu B_\nu &= \frac{1}{2} \tilde{\sigma}^{\mu\nu} (\sqrt{2} n^\mu U_{\nu\mu}^\perp - \sigma_\nu^\mu U_\mu^- - \sigma_\nu^\mu U_\mu^+) (\sqrt{2} \tilde{\sigma}_\mu^\lambda s^\epsilon U_{\lambda\epsilon}^\perp - \tilde{\sigma}_\mu^\lambda U_\lambda^- + \tilde{\sigma}_\mu^\lambda U_\lambda^+), \\ &= \frac{1}{2} \sigma^{\mu\nu} U_\mu^- U_\nu^- - \frac{1}{2} \sigma^{\mu\nu} U_\mu^- \ell^\lambda U_{\nu\lambda}^\perp + \dots, \end{aligned} \quad (4.35)$$

which is a condition of the form

$$(p^\mu U_\mu^-)^2 + (q^\mu U_\mu^-)^2 + A(p^\mu U_\mu^-) + B(q^\mu U_\mu^-) + C = 0, \quad (4.36)$$

for functions  $A$ ,  $B$ , and  $C$  that depend on the characteristic modes  $U_\mu^+$  and  $U_{\alpha\mu}^\perp$  and the desired boundary flux function  $F$ . This is not enough information to gain both components  $(p^\mu U_\mu^-)$  and  $(q^\mu U_\mu^-)$  of the incoming modes. Controlling the Poynting flux gives a one parameter family of solutions for the incoming characteristic modes, so we need a second condition to obtain a unique solution. One way to do this is to control the dot product of the electric and magnetic fields in the boundary surface as well:

$$\sigma^{\mu\nu} E_\mu B_\nu = G(x^\alpha). \quad (4.37)$$

We will interpret this second condition as choosing the polarization of reflected electromagnetic waves, or rather what polarization of electromagnetic waves are injected into the domain in response to the polarization of the incident waves. This second condition gives

$$\begin{aligned} \sigma^{\mu\nu} E_\mu B_\nu &= \frac{1}{2} \sigma^{\mu\nu} (\sqrt{2} n^\mu U_{\nu\mu}^\perp - \sigma_\nu^\mu U_\mu^- - \sigma_\nu^\mu U_\mu^+) (\sqrt{2} \tilde{\sigma}_\mu^\nu U_{\nu\mu}^\perp s^\mu - \tilde{\sigma}_\mu^\nu U_\nu^- + \tilde{\sigma}_\mu^\nu U_\nu^+), \\ &= -\frac{1}{2} \tilde{\sigma}^{\mu\nu} U_\mu^- \ell^\lambda U_{\nu\lambda}^\perp + \dots, \end{aligned} \quad (4.38)$$

which is a condition of the form

$$B(p^\mu U_\mu^-) - A(q^\mu U_\mu^-) + E = 0, \quad (4.39)$$

for some function  $E$  that depends on the characteristics  $U_\mu^+$  and  $U_{\alpha\mu}^\perp$  and the desired polarization function  $G$ . Together, these conditions can be used to obtain the tangential components  $p^\mu U_\mu^-$  and  $q^\mu U_\mu^-$ . Since this is a quadratic system of conditions, there are two solutions given the values of  $A$ ,  $B$ ,  $C$ ,  $D$ , and  $E$ . This is similar to some cases we have encountered before, like the scalar wave equation. Scalar waves that exactly conserve energy at a boundary (i.e. with perfectly reflecting boundary conditions) have two possible boundary conditions, a Dirichlet-type and a Neumann-type condition (see Chapter 2).

One degree of freedom we have left is the choice of the vectors  $p^\mu$  and  $q^\mu$ , we can rotate these unit vectors however we like. One way to define the orientation of this basis is to require

$$p^\mu \ell^\lambda U_{\mu\lambda}^\perp = 0, \quad (4.40)$$

which sets  $A = 0$  in our conditions. This uniquely defines the component  $p^\mu U_\mu^-$ , and the two solutions are

$$p^\mu U_\mu^- = -\frac{E}{B}, \quad q^\mu U_\mu^- = -\frac{B^2 \pm \sqrt{B^2(B^2 - 4C) - 4E^2}}{2B}, \quad (4.41)$$

which we might interpret as a Dirichlet-type or a Neumann-type depending on the  $\pm$  solution chosen.

### 4.3 Einstein's Geometrodynamics

In a similar fashion to electrodynamics, we now work to motivate radiative boundary conditions in Einstein's "geometrodynamics". We will assume the same generalized harmonic formulation and the boundary condition projection formalism introduced in Chapter 3. As was introduced in that chapter, the characteristic modes for the generalized harmonic system were

$$U_{\mu\nu}^+ \equiv k^\alpha \partial_\alpha g_{\mu\nu} = -\frac{1}{\sqrt{2}}(P_{\mu\nu} + s^i d_{i\mu\nu}), \quad (4.42)$$

$$U_{\mu\nu}^- \equiv \ell^\alpha \partial_\alpha g_{\mu\nu} = -\frac{1}{\sqrt{2}}(P_{\mu\nu} - s^i d_{i\mu\nu}), \quad (4.43)$$

$$U_{\alpha\mu\nu}^\perp \equiv \sigma_\alpha{}^\beta \partial_\beta g_{\mu\nu} = \sigma_\alpha{}^i d_{i\mu\nu}. \quad (4.44)$$

This is unfortunately not very applicable in a general fashion, as this definition of the characteristic modes assumes a static worldtube, one where the normal to the timelike hypersurface of the worldtube  $r^\mu$  is purely spatial. This does not need to be the case in general, as the 2-surface can be moving within the 3-space, making  $r^\mu$  point into the future/past, and thus  $n^\mu r_\mu \neq 0$ . The characteristic modes should be defined relative to the worldtube  $\mathcal{B}$  to account for this potential motion. The worldtube hypersurface is defined based on a function  $\Psi(x^\mu) = 0$ , and we will assume this function is given for all time in the simulation. The normal to the hypersurface is constructed as

$$r_\mu = \nabla_\mu \Psi / \psi, \quad (4.45)$$

where  $\psi^2 = g^{\mu\nu} \nabla_\mu \Psi \nabla_\nu \Psi$  is the factor assuring it is a unit vector. The overall sign is chosen such that  $r^\mu$  points out of the manifold  $\mathcal{M}$ . The metric on  $\mathcal{B}$  is given by the projection

$$h_{\mu\nu} = g_{\mu\nu} - r_\mu r_\nu. \quad (4.46)$$

In the same fashion, we construct the timelike unit normal  $n^\mu$  to the constant time slices  $\mathcal{N}_t$  pointing into the future, and the metric on  $\mathcal{N}_t$  is given by

$$\gamma_{\mu\nu} = g_{\mu\nu} + n_\mu n_\nu. \quad (4.47)$$

Where  $\mathcal{B}$  and  $\mathcal{N}_t$  intersect is the constant time 2-surface manifold of the boundary  $S$ . We can construct the purely spatial unit normal to  $S$  by projecting  $r^\mu$  into  $\mathcal{N}_t$  and normalizing:

$$s^\mu \propto \gamma^\mu{}_\nu r^\nu = \frac{r^\mu + (n^\nu r_\nu) n^\mu}{\sqrt{1 + (n^\nu r_\nu)^2}}. \quad (4.48)$$

We can also construct the timelike normal to  $S$  that lies purely within  $\mathcal{B}$ :

$$n_S^\mu \propto h^\mu{}_\nu n^\nu = \frac{n^\mu - (n^\nu r_\nu) r^\mu}{\sqrt{1 + (n^\nu r_\nu)^2}} = \sqrt{1 + (n^\nu r_\nu)^2} n^\mu - (n^\nu r_\nu) s^\mu. \quad (4.49)$$

To make the following analysis more general, we will consider a generic timelike vector field within  $\mathcal{B}$  that is related to  $n_S^\mu$  and  $s^\mu$  as

$$u^\mu = \gamma \left( \sqrt{1 + (n^\nu r_\nu)^2} n^\mu - (n^\nu r_\nu) s^\mu + v^\mu \right), \quad (4.50)$$

where  $v^\mu = \sigma^\mu{}_\nu v^\nu = u^\mu / \gamma - n_S^\mu$  is a vector field tangent to  $S$  that measures the deviation of  $u^\mu$  from  $n_S^\mu$  and  $\gamma^{-2} = 1 - (v^\mu v_\mu)^2$  is a Lorentz factor ensuring  $u^\mu$  is a unit vector. We then use  $u^\mu$  and  $r^\mu$  as an orthonormal Lorentzian basis to construct an ingoing null vector  $\hat{k}^\mu$ , an outgoing null vector  $\hat{\ell}^\mu$ , and the metric of a new 2-surface ( $\hat{\sigma}_{\mu\nu}$ ):

$$\hat{k}^\mu = \frac{1}{\sqrt{2}}(u^\mu - r^\mu), \quad \hat{\ell}^\mu = \frac{1}{\sqrt{2}}(u^\mu + r^\mu), \quad \hat{\sigma}_{\mu\nu} = g_{\mu\nu} + 2\hat{k}_{(\mu}\hat{\ell}_{\nu)}. \quad (4.51)$$

The 2-metric  $\hat{\sigma}_{\mu\nu}$ , being orthogonal to  $u^\mu$  and  $r^\mu$ , is defined relative to a spacelike 2-surface manifold  $S'$  different from  $S$ , as it doesn't necessarily lie on a constant time slice. The various vector fields involved in this construction are visualized in Figure 4.2. It is only when  $v^\mu = 0$  that  $\hat{k}^\mu$  and  $\hat{\ell}^\mu$  are simple rescalings of  $k^\mu$  and  $\ell^\mu$ . We then take these basis vectors and construct the characteristic modes with them:

$$U_{\mu\nu}^+ \equiv \hat{k}^\alpha \partial_\alpha g_{\mu\nu} = -\frac{1}{\sqrt{2}}(a_+ P_{\mu\nu} + b_+ s^i d_{i\mu\nu} - \gamma v^i d_{i\mu\nu}), \quad (4.52)$$

$$U_{\mu\nu}^- \equiv \hat{\ell}^\alpha \partial_\alpha g_{\mu\nu} = -\frac{1}{\sqrt{2}}(a_- P_{\mu\nu} + b_- s^i d_{i\mu\nu} - \gamma v^i d_{i\mu\nu}), \quad (4.53)$$

$$U_{\alpha\mu\nu}^\perp \equiv \hat{\sigma}_\alpha{}^\beta \partial_\beta g_{\mu\nu}, \quad (4.54)$$

where

$$a_\pm = \gamma \sqrt{1 + (n^\nu r_\nu)^2} \mp (n^\nu r_\nu), \quad b_\pm = \gamma(n^\nu r_\nu) \pm \sqrt{1 + (n^\nu r_\nu)^2}. \quad (4.55)$$

We take  $U_{\mu\nu}^-$  as the incoming characteristic modes and endeavor to replace them with boundary conditions, which is still valid as long as the characteristic speed of  $U_{\mu\nu}^-$  is always negative (i.e. propagating into the domain), which is true as long as  $\mathcal{B}$  and  $u^\mu$  remain timelike. Other characteristics like  $U_{\alpha\mu\nu}^\perp$  may be propagating into the domain as well, but the boundary conditions used in place of them are taken to satisfy spatial derivative

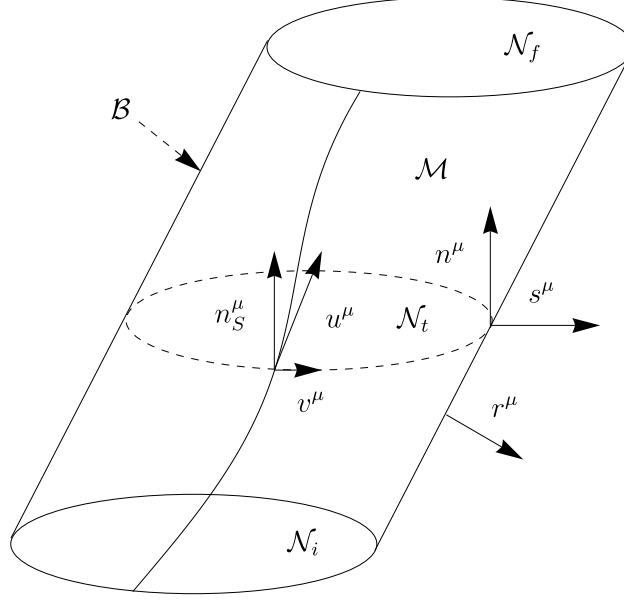


Figure 4.2: Diagram labeling various vectors involved in the quasi-local conservation law construction, where time runs on the vertical, the 3-space is horizontal, and null rays run along  $45^\circ$  lines. The worldtube  $\mathcal{B}$  can be moving with respect to the current time slice  $\mathcal{N}_t$ , as long as the vector orthogonal to it,  $r^\mu$ , remains spacelike. The vector field  $u^\mu$  lies tangent to  $\mathcal{B}$  and follows a curve in  $\mathcal{B}$  to which it is also tangent.

constraints in the system. As in Chapter 3, the components of  $U_{\mu\nu}^-$  are split into constraint, gravitational wave, and gauge groups, but now constructed with the basis  $(\hat{k}^\mu, \hat{\ell}^\mu, \hat{\sigma}_{\mu\nu})$ :

$$\delta_{(\mu}^{(\alpha} \delta_{\nu)}^{\beta)} = \hat{C}_{\mu\nu}^{\alpha\beta} + \hat{P}_{\mu\nu}^{\alpha\beta} + \hat{G}_{\mu\nu}^{\alpha\beta}, \quad (4.56)$$

where the gravitational wave projector is now given as the traceless projection onto  $S'$ :

$$\hat{P}_{\mu\nu}^{\alpha\beta} \equiv \hat{\sigma}_{(\mu}^{(\alpha} \hat{\sigma}_{\nu)}^{\beta)} - \frac{1}{2} \hat{\sigma}_{\mu\nu} \hat{\sigma}^{\alpha\beta}. \quad (4.57)$$

The boundary conditions on the constraint and the gauge groups are unchanged in interpretation and application, just with projections adjusted to the new hatted basis.

### 4.3.1 Radiative Boundary Conditions

We now turn to the family of quasi-local conservation laws introduced in Section 4.1:

$$\partial_t \oint n_\mu^S T_B^{\mu\nu} \psi_\nu dS = \oint \alpha \left[ \frac{1}{8\pi} T^{\mu\nu} r_\mu \psi_\nu - T_B^{\mu\nu} \hat{\nabla}_{(\mu} \psi_{\nu)} \right] dS. \quad (4.58)$$

For what follows, we assume a vacuum spacetime (or at least boundary conditions on all matter fields such that  $T^{\mu\nu} r_\mu \psi_\nu = 0$ ). Consider the choice  $\psi_\mu = u_\mu$ , where  $u_\mu$  is a timelike unit vector field that satisfies a set of dynamical properties and is the same vector field used to construct the characteristic modes in the previous section. We introduce the covariant acceleration of  $u^\mu$ :

$$a^\mu = u^\nu \nabla_\nu u^\mu, \quad (4.59)$$

which dictates its dynamics. As the tensor  $\hat{\nabla}_\mu u_\nu$  makes an appearance in the quasi-local flux terms, we introduce the decomposition

$$\hat{\nabla}_\mu u_\nu = h_\mu^\alpha h_\nu^\beta \nabla_\alpha u_\beta = \frac{1}{2} \theta \hat{\sigma}_{\mu\nu} + \theta_{\mu\nu} + \omega_{\mu\nu} - u_\mu \hat{\sigma}_\nu^\alpha a_\alpha, \quad (4.60)$$

where  $\omega_{\mu\nu} = \hat{\sigma}_{[\mu}^\alpha \hat{\sigma}_{\nu]}^\beta \nabla_\alpha u_\beta$  is the rotation tensor,  $\theta_{\mu\nu} = \hat{P}_{\mu\nu}^{\alpha\beta} \nabla_\alpha u_\beta$  is the shear tensor,  $\theta = \hat{\sigma}^{\mu\nu} \nabla_\mu u_\nu$  is the expansion.

Here, we consider a specific choice of  $u^\mu$  that satisfies the conditions of an Inertial Quasi-local Frame (IQF). This is not the only choice one can make, in principle any frame can be chosen as long as  $u^\mu$  remains timelike and tangent to  $\mathcal{B}$ . In the works [65, 74], along with IQFs, another frame called a Rigid Quasi-local Frame (RQF) is also introduced, which reduces the quasi-local energy flux to a form very similar to the Poynting flux in electrodynamics. The choice of an IQF makes the reflecting boundary conditions more straightforward to derive however, so we will focus on this choice.

An IQF is a choice of observers  $u^\mu$  that has normal acceleration  $r^\mu a_\mu$  such that the expansion vanishes ( $\theta = 0$ ), and vanishing tangential acceleration ( $\hat{\sigma}_\mu^\nu a_\nu = 0$ ). Under such conditions, the quasi-local energy flux simplifies dramatically:

$$T_B^{\mu\nu} \hat{\nabla}_{(\mu} u_{\nu)} = T_B^{(\mu\nu)} \theta_{\langle\mu\nu\rangle} = \frac{1}{4} (\hat{P}_{\mu\nu}^{\alpha\beta} \mathcal{L}_r g_{\alpha\beta}) (\hat{P}^{\mu\nu\epsilon\sigma} \mathcal{L}_u g_{\epsilon\sigma}), \quad (4.61)$$

where we have introduced the notation  $P_{\alpha\beta}^{\mu\nu} T_{\mu\nu}^{\mathcal{B}} = T_{\langle\alpha\beta\rangle}^{\mathcal{B}}$ . The Lie derivative in the  $r^\mu$  direction can be expressed in terms of derivatives of the metric and derivatives of the function  $\Psi$ :

$$\begin{aligned} \hat{P}_{\mu\nu}^{\alpha\beta} \mathcal{L}_r g_{\alpha\beta} &= \frac{1}{2} \hat{P}_{\mu\nu}^{\alpha\beta} \left( r^\lambda \partial_\lambda g_{\alpha\beta} - 2r^\lambda \partial_{(\alpha} g_{\beta)\lambda} + \frac{2}{\psi} \partial_\alpha \partial_\beta \Psi \right), \\ &= \frac{1}{2} \left( \frac{1}{\sqrt{2}} U_{\langle\mu\nu\rangle}^- - \frac{1}{\sqrt{2}} U_{\langle\mu\nu\rangle}^+ - 2r^\lambda U_{\langle\mu\nu\rangle\lambda}^\perp + \frac{2}{\psi} \partial_{\langle\mu} \partial_{\nu\rangle} \Psi \right). \end{aligned} \quad (4.62)$$

Under the IQF conditions, if the vector field  $u^\mu$  is initially hypersurface orthogonal ( $\omega_{\mu\nu} = 0$ ), then it will remain so for all time. We can then express it as proportional to a gradient:

$$u_\mu = \nabla_\mu \phi / \varphi, \quad (4.63)$$

for some function  $\phi$  and a normalization  $\varphi$ . The Lie derivative in the  $u^\mu$  direction takes a similar form:

$$\begin{aligned} \hat{P}_{\mu\nu}{}^{\alpha\beta}(\mathcal{L}_u g_{\alpha\beta}) &= \frac{1}{2} \hat{P}_{\mu\nu}{}^{\alpha\beta} \left( u^\lambda \partial_\lambda g_{\alpha\beta} - 2u^\lambda \partial_{(\alpha} g_{\beta)\lambda} + \frac{2}{\varphi} \partial_\alpha \partial_\beta \phi \right), \\ &= \frac{1}{2} \left[ \frac{1}{\sqrt{2}} U_{\langle\mu\nu\rangle}^- + \frac{1}{\sqrt{2}} U_{\langle\mu\nu\rangle}^+ - 2u^\lambda U_{\langle\mu\nu\rangle\lambda}^\perp + \frac{2}{\varphi} \partial_{\langle\mu} \partial_{\nu\rangle} \phi \right]. \end{aligned} \quad (4.64)$$

To control the quasi-local energy flux we consider a condition

$$T_B^{(\mu\nu)} \hat{\nabla}_{\langle\mu} u_{\nu\rangle} = F(x^\mu), \quad (4.65)$$

for some specified flux function  $F(x^\mu)$ , where  $F(x^\mu) = 0$  is interpreted as a perfectly reflecting condition. The flux specification is a condition of the form

$$(U_+^-)^2 + (U_\times^-)^2 + A(U_+^-) + B(U_\times^-) + C = 0, \quad (4.66)$$

for functions  $A$ ,  $B$ , and  $C$  that depend on the characteristics  $U_{\mu\nu}^+$  and  $U_{\alpha\mu\nu}^\perp$  and the desired boundary flux function  $F$ . Here, the  $+$  polarization component of  $U_{\mu\nu}^-$  is  $U_+^- \equiv (p^\mu p^\nu - q^\mu q^\nu) U_{\mu\nu}^-$  and the  $\times$  polarization component is  $U_\times^- \equiv 2p^{(\mu} q^{\nu)} U_{\mu\nu}^-$ , where  $p^\mu$  and  $q^\mu$  form an orthonormal basis spanning  $S'$ .

Just like the electromagnetic case, we require a second condition that controls the polarization of reflected waves. Motivated by the control of the dot product of the electric and magnetic fields on the 2-surface in the previous section, we can postulate a condition of the form

$$B(U_+^-) - A(U_\times^-) + E = 0, \quad (4.67)$$

for some function  $E$  that depends on the characteristics  $U_{\mu\nu}^+$  and  $U_{\alpha\mu\nu}^\perp$ . With these two conditions, we have a set boundary conditions on the two components of  $U_{\mu\nu}^-$  that we interpret as the gravitationally radiating degrees of freedom. The basis vectors can be rotated in principle to simplify the solutions to these two conditions however desired, but a boundary value for each of the two incoming gravitational wave components given by the projection  $\hat{P}_{\alpha\beta}{}^{\mu\nu} U_{\mu\nu}^-$  can be set as boundary conditions for any choice while controlling the quasi-local flux of gravitational waves.

## 4.4 Conclusion and Future work

In this chapter, we considered setting boundary conditions on the radiating degrees of freedom of gravitational waves based on controlling the energy flux in a quasi-local energy conservation law. We introduced the distinction between local and quasi-local conservation laws by analyzing energy flux based boundary conditions in both Maxwell's electrodynamics and Einstein's geometrodynamics. While setting boundary conditions based on conserving a type of energy can be done, a second condition is needed to set the polarization of the reflected waves. We used electrodynamics to gain some insight into what polarization conditions might make sense to completely determine the incoming components responsible for the radiative degrees of freedom.

As a part of future work, it is important to implement these boundary conditions numerically so that the general stability of such conditions can be rigorously tested. Not only does the numerical stability of such conditions need to be verified, but there may also exist ergoregion and super-radiance instabilities when the boundary is placed close to the horizon of a Kerr black hole. It is not clear yet if applying reflecting boundary conditions will produce such instabilities, and future work will need to address this concern. The quasi-local conservation law framework includes interpretations of energy conservation as well as linear and angular momentum conservation, so it would be interesting to explore what given boundary conditions imply about the change in angular and linear momentum of a Kerr black hole for example, especially in the near extremal spin case.

## Chapter 5

# Conclusion and Future Outlook

In this thesis, a great amount of effort was taken to demonstrate and properly formulate the initial boundary value problem in numerical relativity. The ability to evolve Einstein's field equations with boundaries placed within the strong gravity region of a dynamical spacetime is motivated, considered for a large class of potential boundary conditions, and demonstrated numerically.

This work is motivated by a need to simulate black hole echoes, the reflection of ingoing gravitational and matter waves near the horizon of black holes induced by potential quantum structure. Implementing a reflecting surface near the horizon of a black hole by imposing reflecting boundary conditions there is one way to achieve this. Another motivation is to improve upon the stability and computational efficiency of binary black hole merger simulations by coupling the frameworks presented here with Cauchy characteristic matching techniques. The formulation and numerical framework of the evolution equations we present here allow for the shrinking of the Cauchy domain, leading to dramatically more computationally efficient simulations. One more motivation is the ability to simulate the dynamics of arbitrary compact objects in numerical relativity. Given the time evolution of a boundary surface larger than the horizon of a black hole and the boundary conditions on that surface, any compact object can be simulated in principle with or without assumptions about the interior region of the object.

One aspect of the success shown here comes from analytical tools that guide the specific form of the evolution equations themselves. This includes the concept of symmetric hyperbolicity, where the evolution equations are written in a form that allows for an energy estimate, which when coupled with a proper numerical implementation, can be demonstrated as an approximately bounded quantity of the system.

Another part of the success in these demonstrations comes from implementing modern numerical methods to the system of evolution equations that comprises Einstein’s field equations. We show that summation by parts operators and simultaneous approximation terms can be used to ensure that the energy estimate of the system is approximately conserved even on a discrete grid. We demonstrate the use of a relatively new class of summation by parts methods that allow for arbitrarily shaped domains while using a rectangular grid.

Finally, we developed boundary conditions on the radiative degrees of freedom in the metric by controlling the quasi-local energy flux through the boundary. We showed that gravitational waves are analogous to electromagnetic waves in the sense that two conditions are needed, a conservation of energy and a polarization specifying condition.

## 5.1 Future Work

The work performed in this thesis opens the door to many different directions in numerical relativity. The numerical methods we introduce and demonstrate in Chapter 3 allow for much more complex initial boundary value problems, including

- Non-spherically shaped and non-convex inner boundaries
- Dynamical inner boundaries
- Non-cubical outer boundaries
- Higher accuracy finite differencing operators

Successful evolution of a dynamical boundary would allow for a much simplified binary black hole excision with finite differencing algorithms. The development of an evolution formalism for the worldtube that ties the 2-surface boundary to dynamical black holes would allow for merger simulations with reflecting boundary conditions placed near the horizons of the black holes, which would serve as the first nonlinear simulation of black hole echoes. We plan to study further how such an evolution can be achieved numerically when coupled with the numerical methods we introduced and demonstrated. Coupling these methods with Cauchy characteristic matching techniques would allow for the extraction of gravitational waveforms at null infinity while dramatically improving computational efficiency by reducing the size of the Cauchy domain.

We proposed in this work to use quasi-local conservation laws to define what it means to reflect gravitational radiation, as well as how to interpret what a given set of boundary conditions implies about the mass, linear momentum, and angular momentum within a closed boundary as the system evolves over time. We showed that boundary conditions on the radiating degrees of freedom can be set by choosing the quasi-local energy flux, but that another condition is needed to fully set the polarization of reflected modes. A thorough numerical analysis of these conditions is left for future work, including investigations into the analytical and numerical stability of reflecting boundary conditions based on quasi-local conservation laws.

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# APPENDICES

# Appendix A

## Enclosed Boundary Problem for Cylindrically Symmetric Gravitational Waves

Black hole echoes have been discussed in the literature in the context of both scalar waves and gravitational waves (GWs). Defining reflecting boundary conditions (BCs) in the context of a local mass-energy for scalar waves was done in Section 3.5, but this can also be done for GWs. There are no GWs in the restriction of spherical symmetry, however there are well known examples in the framework of Einstein-Rosen waves [98, 80]. These vacuum solutions use coordinates  $x^\mu = (t, \rho, z, \varphi)$  and have the line element

$$ds^2 = e^{2(\gamma-\psi)} (-dt^2 + d\rho^2) + e^{2\psi} dz^2 + \rho^2 e^{-2\psi} d\varphi^2, \quad (\text{A.1})$$

where  $\psi$  and  $\gamma$  are functions of  $\rho$  and  $t$  only. Einstein's vacuum field equations dictate that  $\psi$  satisfies the cylindrically symmetric wave equation:

$$\partial_t^2 \psi = \partial_\rho^2 \psi + \frac{1}{\rho} \partial_\rho \psi, \quad (\text{A.2})$$

and that the time dependence of  $\gamma$  is dictated by

$$\partial_t \gamma = 2\rho \partial_t \psi \partial_\rho \psi, \quad (\text{A.3})$$

and is subject to the constraint

$$\partial_\rho \gamma = \rho (\partial_\rho \psi)^2 + \rho (\partial_t \psi)^2. \quad (\text{A.4})$$

The local mass-energy of the spacetime is measured with the so-called  $C$ -energy [80], which is simply given by

$$M(\rho, t) = \gamma/4, \quad (\text{A.5})$$

and thus Eqns. (A.3) and (A.4) are proportional to its  $\rho$  and  $t$  derivatives. We can then write the conservation law

$$\partial_t \int_a^b \frac{1}{2} [(\partial_\rho \psi)^2 + (\partial_t \psi)^2] \rho d\rho = \rho \partial_t \psi \partial_\rho \psi \Big|_a^b, \quad (\text{A.6})$$

which happens to be identical to the conservation law for the cylindrically symmetric wave equation outside of the context of general relativity. The BCs that keep the  $C$ -energy from changing are then given by the classical Dirichlet/Neumann conditions  $\partial_t \psi = 0$  and  $\partial_\rho \psi = 0$ . We can then define a reflecting IBVP as we did in spherical symmetry. The BCs are simple due to the gauge fixed assumption of the line element considered here, but this may not be the case if a more general line element where the “perimeter radius”  $\rho$  is allowed to be dynamic, as it was in our dynamic examples in spherical symmetry.

## Appendix B

### Static scalar field Summation By Parts

The Klein-Gordon equation  $\nabla^\mu \nabla_\mu \phi - m^2 \phi = 0$  can be reduced to a first order system with the definition of two different auxiliary variables than those considered in the main text:  $\Pi \equiv \partial_t \phi$  and  $\psi^i \equiv [(\alpha^2 - \beta_j \beta^j) \partial^i \phi + \beta^i \partial_t \phi] / \alpha$ . The evolution equations in spherical symmetry for a static background look particularly simple,

$$\partial_t \phi = \Pi, \quad (\text{B.1})$$

$$\partial_t \psi^r = \beta^r \nabla_r \psi^r + \alpha \partial^r \Pi - m^2 \alpha \beta^r \phi, \quad (\text{B.2})$$

$$\partial_t \Pi = \alpha \nabla_r \psi^r + \beta^r \partial_r \Pi - m^2 \alpha \phi, \quad (\text{B.3})$$

where  $\nabla_r \psi^r = (\sqrt{\gamma})^{-1} \partial_r (\sqrt{\gamma} \psi^r)$  is the 3-divergence. This system of equations admits the following conservation law as long as  $c_+ c_- < 0$  throughout the domain:

$$\begin{aligned} \partial_t \int_a^b \frac{1}{2} \left( \frac{\alpha \Pi^2 + \alpha \psi_r \psi^r - 2 \psi_r \beta^r \Pi}{(\alpha^2 - \beta_r \beta^r)} + m^2 \phi^2 \right) \sqrt{\gamma} dr \\ = \Pi \psi^r \sqrt{\gamma} \Big|_a^b. \end{aligned} \quad (\text{B.4})$$

Distributing the time derivative and substituting the evolution equations, we obtain

$$\int_a^b \Pi \nabla_r \psi^r \sqrt{\gamma} dr + \int_a^b (\partial_r \Pi) \psi^r \sqrt{\gamma} dr = \Pi \psi^r \sqrt{\gamma} \Big|_a^b. \quad (\text{B.5})$$

Crucially, the definition of the auxiliary variables  $\Pi$  and  $\psi^r$  make the flux term on the right hand side a simple multiple of the two variables and Eq. (3.6) is in exactly the same form

as Eq. (2.61), which will set up the problem to be directly mimicked by the covariant SBP property when  $\Pi$  and  $\psi^r$  become grid functions:

$$\Pi^T W \nabla \psi^r + (D\Pi)^T W \psi^r = \Pi \psi^r \sqrt{\gamma} \Big|_a^b, \quad (\text{B.6})$$

where the operator  $\nabla \equiv \Gamma^{-1} D \Gamma$  approximates the covariant 3-divergence of 3-vectors, the operator  $D$  approximates the covariant scalar gradient, and  $W \equiv \Sigma \Gamma$  is the covariant norm operator and approximates covariant integration.

# Appendix C

## Discrete Closed Surface Integration

In order to calculate quasi-local quantities such as the Hawking mass, we require a way to approximate surface integrals on the embedded boundaries in our domain. This integration scheme must be compatible with the rectangular nature of the grid used in the numerical methods we consider in this work. One can express an integral over a convex closed surface  $S$ , defined by the function  $\phi(x^i) = 0$ , with integrand  $f(x^i)$ , as two 2D region integrals:

$$\oint f dS = \int_{X^\pm} f[x(y, z), y, z] \sqrt{\sigma} dy dz, \quad (\text{C.1})$$

where the region  $X^\pm$  is the projection (or shadow) of the closed surface onto the  $y$ - $z$  plane and the  $\pm$  indicates the inclusion of both the projections from the  $\pm x$  sides of the surface. The function  $x(y, z)$  is the expression  $\phi(x^i) = 0$  solved for  $x$ , which will have two solutions for a convex closed surface corresponding to the  $\pm$  projections. The 2-metric determinant  $\sigma$  is determined by projecting the 2-metric

$$\sigma_{ij} = \gamma_{ij} - s_i s_j, \quad (\text{C.2})$$

onto the  $y$ - $z$  plane. The projection operator onto the 2-surface is given by

$$e_{\mathcal{A}}^i = \frac{\partial x^i}{\partial \theta^{\mathcal{A}}}. \quad (\text{C.3})$$

In this example, we choose the coordinates on the  $y$ - $z$  plane as  $\theta^{\mathcal{A}} = (y, z)$  so that  $e_{\mathcal{A}}^i = (\partial_{\mathcal{A}} x(y, z), \delta_{\mathcal{A}}^y, \delta_{\mathcal{A}}^z)$ . The projected 2D metric is given by

$$\sigma_{AB} = e_{\mathcal{A}}^i e_{\mathcal{B}}^j \sigma_{ij}. \quad (\text{C.4})$$

We then take the determinant to find the surface area element  $\sqrt{\sigma}$  and integrate the integrand and the surface area element over the 2D regions  $X^\pm$ . An appropriate quadrature rule can then be chosen to perform this integral in approximation on a finite number of sampled points, as is defined for our numerical method in [67]. Since we also have independent grid intersections with the  $Y^\pm$  and  $Z^\pm$  projection directions, we can repeat the surface integral three times, and average them to get a more accurate result.

# Appendix D

## Spherical Kerr-Schild

A spinning black hole can be described in traditional Kerr-Schild coordinates, but this has the disadvantage that the horizons are oblate ellipsoids in coordinate space, which makes the problem of excision more complicated. However, with the aid of a coordinate transformation detailed in [73], the horizons can instead take on a spherical shape in coordinate space. Using the coordinates  $x^\mu = (t, x, y, z)$ , this metric can be expressed in the usual Kerr-Schild form:

$$g_{\mu\nu} = \eta_{\mu\nu} + 2Hl_\mu l_\nu, \quad (\text{D.1})$$

with

$$H = \frac{Mr^3}{r^4 + a^2 z^2}, \quad R^2 = \frac{(r^4 + a^2 z^2)}{(r^2 + a^2)}, \quad (\text{D.2})$$

and

$$l_\mu = \left(1, \frac{xR^2}{r^3} + \frac{ay}{r^2}, \frac{yR^2}{r^3} - \frac{ax}{r^2}, \frac{zR^2}{r^3}\right). \quad (\text{D.3})$$

While  $\eta_{\mu\nu}$  is a representation of Minkowski space, it is not diagonal in these coordinates. It is however diagonal using a traditional transformation to spherical coordinates, so we can construct it with the following set of orthonormal basis vectors:

$$t_\mu = (1, 0, 0, 0), \quad (\text{D.4})$$

$$r_\mu = (0, x, y, z)/A, \quad (\text{D.5})$$

$$\theta_\mu = (0, -xz, -yz, x^2 + y^2)/B, \quad (\text{D.6})$$

$$\varphi_\mu = (0, -y, x, 0)/C, \quad (\text{D.7})$$

with

$$A^2 = \frac{r^4(r^2 + a^2)}{r^4 + a^2 z^2}, B^2 = \frac{r^6(x^2 + y^2)}{r^4 + a^2 z^2}, C^2 = \frac{r^2(x^2 + y^2)}{r^2 + a^2}, \quad (\text{D.8})$$

and

$$\eta_{\mu\nu} = -t_\mu t_\nu + r_\mu r_\nu + \theta_\mu \theta_\nu + \varphi_\mu \varphi_\nu, \quad (\text{D.9})$$

taking care that a smooth limit to the diagonal metric  $\eta_{\mu\nu} = \text{diag}(-1, 1 + (a/z)^2, 1 + (a/z)^2, 1)$  is attained when  $x = y = 0$ .