APPLICATION OF METHODS FROM NUMERICAL RELATIVITY TO LATE-UNIVERSE COSMOLOGY

JAMES B. MERTENS

Submitted in partial fulfillment of the requirements for the degree of

Doctor of Philosophy

Dissertation Adviser: Prof. Glenn D. Starkman

Department of Physics

CASE WESTERN RESERVE UNIVERSITY

January 2017
We hereby approve the dissertation of

James B. Mertens

candidate for the degree of Doctor of Philosophy*

Committee Chair

Glenn D. Starkman

Committee Member

John ‘Tom’ Giblin

Committee Member

Craig J. Copi

Committee Member

Longhua Zhao

Date of Defense

November 17th, 2016

*We also certify that written approval has been obtained for any proprietary material contained therein.
Contents

List of Figures ii

1 Introduction 1

1.1 General Relativity 5

1.1.1 The Einstein Field Equations 7

1.2 Numerical Formulations of General Relativity 9

1.3 Numerical Relativity in Cosmology 11

2 The BSSNOK Formulation 16

2.1 The 3+1 / ADM Formulation 17

2.1.1 FLRW in 3+1 21

2.2 The BSSNOK Formulation 22

2.3 Reference Metric Formulation 24

2.4 Algebraic Constraint Enforcement 27

2.5 Stability and Constraint Violation Growth 30

3 Cosmological Settings 35

3.1 Pressureless Fluid Dynamics 36
List of Figures

1.1 Stability of the BSSNOK formulation .......................... 3

1.2 Illustration of a Cosmological Spacetime ....................... 15

4.1 Illustration of Geodesic Integration Through a Spacetime ...... 47

5.1 Simulation Inheritance Diagram ................................. 63

5.2 Simulation collaboration diagram ............................... 65

5.3 4th-order Runge Kutta Implementation ....................... 67

5.4 Strong Code Scaling ........................................... 68

5.5 Cosmological Dust Simulation Convergence Test ............... 73

5.6 AwA Stability Test ............................................. 76

5.7 AwA Linear Wave Test ......................................... 79

5.8 AwA Linear Wave Test ......................................... 80

5.9 AwA Linear Wave Test ......................................... 81

5.10 FRW Optical Integration Tests ................................. 82

5.11 Optical Integration through Kasner ........................... 85

5.12 Optical Integration through Kasner ........................... 88
6.1 Variation of Metric Statistics As Spectrum Cutoff Frequency Varies . 95
6.2 Variation of Metric Statistics As Spectrum Amplitude Varies . . . . . 96
6.3 Error in Cosmological Simulations as Resolution Varies . . . . . . . . 99
6.4 Accuracy of the Background FLRW Integrator . . . . . . . . . . . . . 100
6.5 Comparison of a Cosmological Run to Linear Theory . . . . . . . . . 100
6.6 A Standard Hubble Diagram . . . . . . . . . . . . . . . . . . . . . . . 102
6.7 Residual Hubble Diagrams . . . . . . . . . . . . . . . . . . . . . . . . 104
6.8 Violation of Assumptions in the Dyer-Roeder Approximation . . . . . 106
List of Tables

1.1 Formulations of Numerical Relativity . . . . . . . . . . . . . . . . . . 12
One of the biggest challenges to our current understanding of fundamental physics is the unknown matter-energy content of the universe. Thought to be dominated by dark energy and dark matter, a variety of models have arisen attempting to describe these components, with possible explanations ranging from modifications to the theory of general relativity to hypothetical fields driving the accelerated expansion of the universe. As new theories are developed to describe the underlying physics of dark energy and dark matter, increasing levels of precision and accuracy are required from both theoretical predictions and observational data in order to differentiate between various models.

Numerical simulations enable predictions with sub-percent-level accuracy to be extracted from these theories and compared to observations. However, developing sufficiently realistic numerical models requires the consideration of a wide range of physical effects, including gravitational interactions and stress-energy sources. This thesis presents new tools for modeling gravitational effects using the full theory of general relativity, with the goal of enabling the determination of a correct model of fundamental dark sector physics.

In this work, a novel formulation of general relativity is developed and applied in a cosmological setting. A code developed to numerically evolve this formulation
is presented in detail. A demonstration of the code’s ability to accurately model cosmological dynamics is included as a proof of concept, illustrating the potential of this approach to predict observable consequences of gravitational interactions with unprecedented accuracy.
Chapter 1

Introduction

Since the development of the Einstein field equations of general relativity in 1915, a fundamental objective of physics has been to explore and characterize the solutions to these equations. The Einstein field equations describe the behavior of matter in a curved spacetime and how that matter curves spacetime itself – an idea from which the fundamental force of gravitation can be seen to arise. A deeper understanding of the theory has become essential for areas of physics in which gravitational effects are important. In a cosmological setting, the framework of general relativity can be used to test various models that aspire to describe the behavior of the Universe at the largest observable scales, where the unexplained phenomena of dark matter and dark energy dominate the dynamical behavior of the system. Attempts to model these phenomena typically rely on approximate methods to obtain solutions to the Einstein equations. However as the field enters an era of precision cosmology, modeling sub-percent level effects will be necessary in order to obtain predictions accurate enough to compare to observations.
The complexity of the Einstein field equations and the dynamical systems to which they are applied makes obtaining general analytic solutions intractable. Rather, it becomes necessary to adopt a numerical approach, where solutions are obtained at discrete points, and approach a continuum solution in the limit of infinite resolution. Attempts to solve the Einstein field equations on a computer date back nearly to the dawn of general-purpose, transistorized computing itself. Beginning in 1958, and formally publishing in 1964, Susan Hahn and Richard Lindquist created a manuscript detailing the computational modeling of the fully relativistic interaction of two gravitationally bound black holes [1]. Although of significance, subsequent numerical studies did not appear until a decade later in 1975, when Smarr and Eppley used an axi-symmetric code to model gravitational wave production due to interacting black holes [2]. Shortly thereafter, such publications became more common, modeling symmetric spacetimes in order to make the most of the computational resources available at the time.

These early studies were based on a formulation of Einstein’s equations devised by Arnowitt, Deser, and Misner (ADM) [3]. However, the computational work based on this formulation suffered from numerical instabilities. For example, simulations of binary black hole systems would break down before a single orbit could be completed. In 1987, Nakamura, Oohara, and Kojima began using a modified version of the ADM formulation [4–6] that demonstrated substantially improved numerical stability. However, this reformulation was not widely used until it was systematically compared with the standard ADM formulation, and the improvement was demonstrated by Baumgarte and Shapiro in 1998 [7], shown in Figure 1.1.
Figure 1.1: A plot by Baumgarte and Shapiro \cite{7} demonstrating stability of the BSSNOK system. Solutions for a component of the extrinsic curvature for a linearized gravitational wave are presented in two formulations, the ADM (dashed) and BSSNOK (solid). Use of the ADM system is seen to result in unstable evolution.

Due to the development of such stable formulations and improvements in computing resources, the field of numerical relativity has grown into a mature state in which physically realistic systems can be modeled with a high degree of precision. These advances, along with techniques for handling singularities in strongly gravitating regimes, have been applied to a large number of systems, ranging from characterizing properties of black holes in higher dimensions, to precisely predicting the gravitational waveforms from black hole mergers \cite{8,10}.

These developments in numerical relativity are complimented by techniques from the field of cosmology, which make heavy use of N-body simulations in a Newtonian gravity approximation. These techniques, developed independently from the advance-
ments in numerical relativity, model the dominant matter component of the Universe using gravitationally interacting particles. Numerical work evolving with a Newtonian N-body system was first performed in 1960 by von Hoerner [11], who simulated 16 masses. The relevant numerical methods have been heavily developed since this time, progressing to simulations with $10^{12}$ or more particles [12–14]. A substantial amount of effort has been devoted to solving these equations in a scalable and highly parallelizable way.

Although unprecedented in scale and precision, these cosmological simulations rely on a Newtonian approximation. This is justifiable when the amplitudes of metric fluctuations are small on distance scales compared to density scale of the problem, and when the dynamics of the system are well-described by only scalar degrees of freedom. In a late-Universe cosmological setting, these standards are met to a high degree of accuracy [15]. However, a natural question remains surrounding the breakdown of this approximation, and the importance of the neglected effects in a Newtonian or perturbative approach. If observable, such deviations would provide evidence for the validity of general relativity or alternative theories on scales where these effects are important. In order to differentiate between the two in a cosmological setting, such effects will need to be characterized.

This question has received limited attention from the mainstream numerical cosmology and numerical relativity communities. This can be attributed to a number of factors, including a lack of data with the precision necessary to robustly examine effects present in a fully relativistic setting, and perhaps due to the perceived difficulty of employing Einstein’s equations in this context. However, as the quantity and
quality of such datasets increases\cite{16,17} the former of these issues can be alleviated. Furthermore, the development of stable numerical schemes able to resolve all relevant length scales addresses concerns surrounding the tractability of the problem.

The generality with which formulations of numerical relativity have been developed makes them well-suited for the exploration of cosmological systems. Numerical relativity code have not only been used to model collisionless matter, but more general (magneto-)hydrodynamical systems of significant complexity. Indeed, such software has been used to study astrophysical phenomena over a wide range of scales, including mergers of compact objects, physical processes in the early universe, and the dynamics of other strongly gravitating systems. The numerical formulations of general relativity have therefore been validated to an exceptional degree of accuracy and precision; however, the use of these techniques for studying the dynamics of cosmological systems has been limited in quantity and scope. The goal of this thesis is to present a formulation and corresponding code specifically intended to examine the applicability of techniques from numerical relativity to cosmology. The details of the code implementation and the preliminary results it has been used to obtain are also presented.

1.1 General Relativity

A number of ideas and notation from general relativity will be used throughout this work. General relativity aspires to describe aspects of classical physics in a unified manner, based on the idea that dimensions of space and time can be described within
a single, geometric framework. The resulting concept of a ‘spacetime’ is quantitatively described by a 16-component symmetric metric tensor, notated as $g_{\mu\nu}$, with $\mu, \nu \in \{0, 1, 2, 3\}$. It is used to describe how distances are computed at a given location in a spacetime. The length of an infinitesimal spacetime vector $dx^\mu$ is calculated accordingly as

$$ds^2 = g_{\mu\nu}dx^\mu dx^\nu,$$  \hspace{1cm} (1.1)

where the Einstein summation convention is used to denote a sum over $\mu$ and $\nu$. Conventional notation will be utilized here, with Greek letter indices denoting spacetime indices, lowercase Latin letters such as $a$ representing indices in arbitrary dimension, and Latin letters at and after ‘i’ representing spatial indices (eg, $i \in \{1, 2, 3\}$).

The inverse metric is written as $g^{ab}$, so that $g_{ac}g^{cb} = g_a^b = \delta_a^b$. Partial derivatives may be written as $\partial_a F = F,a$, and covariant derivatives as $D_a F = F,a$, where

$$D_a F_{b_1b_2...} = \partial_c F^c_b + \Gamma^{c}_{ab} F^{d_1d_2...}_{b_1b_2...} + \Gamma^{c}_{ad} F^{a_1d_{1}...}_{b_1b_2...} + ... - \Gamma^{d}_{c_1b_1} F^{a_1a_2...}_{d_1b_2...} - \Gamma^{d}_{c_2b_2} F^{a_1a_2...}_{b_1d_{1}...} - ...$$  \hspace{1cm} (1.2)

The above Christoffel symbols are given by

$$\Gamma^c_{ab} = \frac{1}{2} g^{cd} (g_{da,b} + g_{db,a} - g_{ab,d})$$  \hspace{1cm} (1.3)

The ‘mostly-plus’ convention for spacetime indices, or the ($-+++$) signature, will be adhered to in this work, so that the sign of $\text{det}(g_{\mu\nu}) \equiv g$ is negative. Additionally, geometrized units will be used, where the speed of light and gravitational constant
are set to unity, \( c = G = 1 \).

1.1.1 The Einstein Field Equations

An action for the Einstein field equations can be derived elegantly for a \( 3 + 1 \)-dimensional spacetime based on a remarkably simple set of postulates [18]. Stated concisely, these are: 1) physical laws should be invariant under general coordinate transformations; 2) the equations of motion should be second order; and 3) there exists a frame of reference in which the metric looks locally flat, or the local metric is \( g_{\mu\nu} = \text{diag}(-1, 1, 1, 1) \). The resulting action contains what is referred to as an ‘Einstein-Hilbert’ term, which is simply the Ricci scalar,

\[
S = \int d^4x \sqrt{-g} \left\{ \frac{1}{16\pi} R + \mathcal{L}_m \right\} .
\] (1.4)

Here, \( \mathcal{L}_m \) is the Lagrangian describing the matter content of the Universe (which taken to include a cosmological constant here), and the Ricci scalar is the fully contracted Ricci tensor, a tensor describing the geometric curvature at a given location, computed in an arbitrary dimension by \( R = g^{ab} R_{ab} \). The Ricci tensor is in turn a contraction of the Riemann curvature tensor, \( R_{ab} = R^c_{acb} \) which is in turn given by

\[
R^c_{eb} = \partial_a \Gamma^c_{eb} - \partial_b \Gamma^c_{ea} + \Gamma^e_{ad} \Gamma^d_{eb} - \Gamma^e_{bd} \Gamma^d_{ea} .
\] (1.5)

Varying the Einstein-Hilbert action with respect to the metric results in the Ein-
stein field equations, which describe the evolution of the metric in the spacetime,

\[ R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu} = 8\pi T_{\mu\nu}. \] (1.6)

The stress-energy tensor \( T_{\mu\nu} \) comes from varying the matter Lagrangian with respect to the metric.

The Einstein field equations presented here constitute the unique set of second-order equations for the metric components, up to a cosmological constant term [19,20] (which can be considered to be part of the matter Lagrangian). These equations have provided an exceptionally accurate description of the Universe, and have been validated by a wide range of astrophysical phenomena and terrestrial experiments. Nevertheless, it is not a unique theory of gravity: a wide variety of alternative formulations have been developed in an attempt to describe dynamical processes for which no definitive physical model yet exists, particularly the physics of dark energy and dark matter [21].

Although such theories are of interest, exploring them is beyond the scope of this work. However, it is worthwhile to note that numerical relativity can hope to examine any formulation in which the modifications can be written as an effective stress-energy contribution to the equations of motion. In this form, the equations of motion are

\[ R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu} = 8\pi T_{\mu\nu} + S_{\mu\nu} \] (1.7)

and \( S_{\mu\nu} \) contains no second-order time derivatives of the metric.
It will also be important to consider the behavior of test particles in a spacetime, either massive or massless. Perhaps the simplest way of deriving an equation of motion for the paths particles follow is to note that such paths should be ‘straight lines’ when there are no non-gravitational interactions. In this context, a straight line can be considered any path along which the vector tangent to the path is parallel transported. For such a path \(x^\mu(\lambda)\), the tangent will be \(V^\mu \equiv dx^\mu/d\lambda\); along this path the tangent should not change, so that

\[V^\mu \nabla_\mu V^\nu = 0.\]  
(1.8)

Writing the derivative in the direction of propagation as \(V^\mu \partial_\mu \equiv d/d\lambda\), the geodesic equation follows immediately from Eq. (1.8):

\[
\frac{d^2 x^\nu}{d\lambda^2} + \Gamma^\nu_{\alpha\beta} \frac{dx^\alpha}{d\lambda} \frac{dx^\beta}{d\lambda} = 0.
\]  
(1.9)

### 1.2 Numerical Formulations of General Relativity

Many formulations have been developed to solve Einstein’s equations numerically, enabling a diverse set of checks and tests, with each formulation able to validate results from others. A number of these formulations will be described in this section. A significant subset of these are based on the original 3+1, or ADM formulation of general relativity, which describes a spacetime as a set of spatial slices with some timelike separation. While work on such formulations dates back to at least 1927.
the ADM formulation sought to generalize and apply such ideas. The seminal work was published in 1959 \cite{ADM}, quickly found numerous applications. A republication of an original review of the material can be found in Ref. \cite{23}. Notably, the ADM formulation commonly used in numerical relativity is actually a reformulation by York of the original work \cite{24}.

Of particular importance to numerical communities is the BSSNOK formulation \cite{4,5,7}, which not only sees widespread use in numerical relativity, but is also used in this thesis. Chapter 2 provides a more in-depth discussion of this formulation. It is similar to the ADM formulation in that it relies on a 3+1 split, and evolves a spatial metric. However additional auxiliary variables are also evolved in this formulation for added numerical stability. The particular choice of spatial slices – or gauge – is important for numerical stability in this system. In particular, gauges should be chosen where singularities (either coordinate or physical) are neither formed nor resolved. The BSSNOK formulation has been used to study dynamics of a wide variety of cosmological systems, some of which are detailed in Sec. 1.3.

While the BSSNOK formulation has been employed with great success, additional formulations have appeared attempting to further improve numerical stability and minimize violation of the Hamiltonian and momentum constraint equations. Some commonly employed reformulations include the CCZ4, related Z4c, and $C^2$-Adjusted schemes. While these have been demonstrated to do an excellent job minimizing constraint violation in the system, the evolution does not always correspond more closely than the original BSSNOK system to physical, continuum-limit solutions.

While many such formulations are conceptually motivated by a similar 3+1 split-
ting of the Einstein field equations, this is not always the case. A wide range of formulations have arisen through the years as various groups have pursued stable schemes to numerically evolve strongly gravitating systems. Closely related to the CCZ4 formulation is the generalized harmonic formulation, which was developed independently, but is also widely used. This formulation does not begin by performing a 3 + 1 split, but rather by writing down Einstein’s equations subject to a specific gauge condition (harmonic gauge). First written by Friedrich in 1985 \[25\] and later posed in a form more suitable for numerical use \[26\], this formulation was recognized as capable of long-term evolution. Indeed, the first long-term numerical evolution of a binary black system including a merger by Pretorius in 2005 \[8\] uses this formulation. It has since been used to evolve strongly gravitating systems with an exceptional degree of stability.

Many other novel formulations have also been developed. Although it would be beyond the scope of this thesis to try to describe all of them, a partial list can be found in Table 1.1. The majority of these methods attempt to resolve issues near singularities, either coordinate or physical, with a clever choice of variables or coordinate system.

1.3 Numerical Relativity in Cosmology

Literature applying numerical relativity to cosmology date backs to the 1980s, with much of the focus on early-universe phenomena \[27\]. In particular, these works examined physical regimes where nonlinear general relativistic effects are expected to
<table>
<thead>
<tr>
<th>Formulation Name</th>
<th>References</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ADM</td>
<td>3, 24</td>
<td>The ‘original’ 3 + 1 decomposition, divides spacetime into spatial slices described by a 3-metric with time-like separation.</td>
</tr>
<tr>
<td>BSSNOK</td>
<td>4–7</td>
<td>A conformal decomposition of the ADM formulation with additional auxiliary variables. Perhaps the most widely utilized numerical formulation.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Variants of this method include ‘first-order’ reformulations and additions of constraint damping terms (CCZ4 35, Z4c 36, C2-Adjusted 37).</td>
</tr>
<tr>
<td>Generalized Harmonic Coordinates</td>
<td>26, 38</td>
<td>A decomposition in which contracted Christoffel symbols are chosen to be sourced by gauge functions, and Einstein’s equations are written in terms of these functions.</td>
</tr>
<tr>
<td>Einstein-Christoffel Systems</td>
<td>26, 39</td>
<td>A first-order formulation in which the metric and a combination of Christoffel symbols is evolved.</td>
</tr>
<tr>
<td>Characteristic IVP</td>
<td>40, 41</td>
<td>A decomposition of Einstein’s equations onto null hypersurfaces rather than spatial, found in studies of gravitational radiation.</td>
</tr>
<tr>
<td>Tetrad formulations</td>
<td>42, 43</td>
<td>A tetrad-based formulation, where tetrads (effectively, the square root of the metric) are evolved rather than the metric itself.</td>
</tr>
<tr>
<td>Regge Calculus</td>
<td>44, 45</td>
<td>A lattice formulation in which the spacetime is decomposed into ‘4-simplices’ (the 4-dimensional generalization of tetrahedra). Vertex locations and deficit angles at vertices are evolved.</td>
</tr>
</tbody>
</table>

Table 1.1: Formulations of numerical relativity.
be appreciable. Such systems include the pre-inflationary universe, including the problem of determining the initial conditions required for inflation \[28\], and nucleosynthesis in an inhomogeneous universe \[29\]. More general gravitational effects such as nonlinear wave propagation and gravitational soliton solutions were also examined in a cosmological context at this time. \[30-33\] The application of full general relativity to realistic late-universe cosmologies received more limited attention, as Newtonian N-body simulations were considered sufficient for resolving much of the phenomenology. Not until the late 1990’s did a fully relativistic code appear with the intent to more seriously consider late-universe cosmology in a realistic setting \[34\].

Simulations of early universe cosmology in full GR have progressed in recent years, decreasing the restrictions on allowed symmetries and assumptions, and increasing the accuracy and range of parameter space explored in simulations of phenomena ranging from inflationary initial conditions \[46, 47\] to phase transitions \[48-50\]. Applications to late-universe cosmology have also been explored, with studies predominantly falling into two categories: the evolution of toroidal vacuum spacetimes containing a number of singularities – black hole lattices \[51-55\], and studies utilizing matter sources, in the form of a pressureless perfect fluid \[56, 62\] (as depicted in Fig. 1.2) or a scalar field \[63, 64\] mimicking dark matter.

Until recently \[62\], the focus of these studies has been on examining properties of metric components rather than observable consequences. The metric quantities themselves are gauge-dependent, and so will not remain the same under a coordinate transformation or re-foliation of the spacetime. Thus, in general it is desirable to compute observable quantities in order to best compare models to any observations.
It is also important to phrase questions themselves in a fully relativistic language. Much of the intuition in modern cosmology relies on calculation of quantities in perturbation theory. This is sufficient at leading order, where gauge-invariant fields can be uniquely constructed. In principle, corrections to perturbative or Newtonian quantities from a fully relativistic treatment can be explored by computing such quantities. However, interpretations from perturbative cosmology do not apply in a fully relativistic setting. Power spectra of metric variables (even ones that are locally gauge-independent) are also unphysical, not only because they will be foliation-dependent measures, but because Fourier transforms are not well-defined in a curved space. Thus, questions regarding the nature of the spacetime should be posed purely in terms of quantities that are directly measurable – such as number counts, redshifts, intensities, or angular positions – and conclusions about properties of spacetimes drawn from these. This thesis adheres to this idea by computing quantities as would be measured by particular observers in a given spacetime using the full framework of general relativity.

The remainder of this thesis is divided into six chapters. In Chapter 2 the BSS-NOK formulation is motivated and described. A modification is then introduced that is unique to this work, with the intent of reducing numerical error due to a dominant FLRW cosmology. Additional modifications attempting to minimize any constraint violation are also described. In Chapter 3 choices of fully relativistic gauges, initial conditions, and matter sources useful for examining dust cosmologies are described. While these choices have drawn heavily from existing literature, in this work they are tailored to a cosmological setting. Following in Chapter 4 is a discussion of the
geometric optics formalism, used to propagate beams of light through general spacetimes, and which can be used to infer measurable properties of the spacetime. The formulation is then tailored to a useful gauge – geodesic slicing – and reduced to a form tractable for a 3 + 1 numerical code. Chapters 5 and 6 comprise the main numerical work done for this thesis, including implementation details of a code for solving the equations introduced in previous chapters, tests of this code, and preliminary results. Finally, a summary of this work, outlook for this approach, and plans for future developments are explored in Chapter 7.

Figure 1.2: An illustration of a 2-dimensional slice through an inhomogeneous spacetime. Lighter colors represent regions of the spacetime with more matter – denser regions – while darker regions represent regions with less matter.
Chapter 2

The BSSNOK Formulation

As introduced in Ch. 1, numerical attempts to directly integrate the ADM equations quickly break down for many spacetime configurations. While early attempts to correct this relied on a phenomenological approach, mathematical analyses of the equations suggested a specific issue: the ADM formulation is not well-posed, with the exception of several special coordinate systems. This implies that the evolution equations are not guaranteed to produce solutions, or that solutions may not vary smoothly with the initial data [26].

Addressing this issue required a reformulation of the ADM equations. (For a more thorough introduction to these concepts, see [65] or [66].) Many of the formulations of numerical relativity exist to address such problems with stability. Of these, the BSSNOK formulation has demonstrated a substantial degree of success, particularly for several choices of gauge. As a result, this formulation is commonly used in a wide variety of settings.

This formulation is described below, followed by a ‘reference formulation’ that is
unique to this thesis. This modification tailors the BSSNOK formulation to a cosmological setting, attempting to mitigate numerical error by evolving differences from a dominant overall cosmology. Additional modifications to the BSSNOK equations that attempt to mitigate constraint violation are also considered, including a modification to the equation of motion for the extrinsic curvature $K$ that is perhaps unique to this thesis.

### 2.1 The 3+1 / ADM Formulation

The BSSNOK formulation is built upon ideas from the ADM formulation. In the version of the ADM formulation introduced by York, the metric is decomposed into spatial foliations with a timelike separation. A timelike unit vector field normal to the spatial slices, $n^\mu$, is typically written in component form as

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

(2.1)

Because this vector has unit norm and is timelike in the ADM formulation ($n^\mu n_\mu = -1$), the covariant form of the vector can be written as $n_\mu = (-\alpha, 0^i)$. An operator projecting spacetime quantities onto spatial slices can be constructed using this vector,

$$P^\mu_\nu = \delta^\mu_\nu + n^\mu n_\nu.$$

(2.2)

When this projection operator acts on a quantity, the component parallel to $n^\mu$ will be projected out. The metric itself can be projected onto spatial slices, resulting in
the metric ‘induced’ on a spatial hypersurface. Performing this projection,

\[ P_\alpha^\mu P_\beta^\nu g^{\alpha \beta} = P^{\mu \nu}, \]  

(2.3)

demonstrates that the projection operator itself is simply the spatial metric. By projecting the Einstein equations themselves, a set of evolution equations for the spatial metric can be obtained.

Using the variables and relationships described above, the full 4-metric can be written in terms of the spatial metric. Denoting the spatial components as \( \gamma_{ij} \equiv P_{ij} \) and using Eq. 2.2, the metric is given by

\[
g_{\mu \nu} = \begin{pmatrix}
-\alpha^2 + \gamma_{lk} \beta^l \beta^k & \beta_i \\
\beta_j & \gamma_{ij}
\end{pmatrix}.
\]  

(2.4)

The components of the normal \( n^\mu \) are now physically meaningful. The variable \( \alpha \) is referred to as the ‘lapse’, and \( \beta_i \) the ‘shift’, respectively corresponding to the rate at which proper time passes (or amount of time elapsed between 3-surfaces) and an observer’s choice of coordinates on the spatial slices. The parameters \( \alpha \) and \( \beta_i \) are taken to encompass all four gauge degrees of freedom.

The extrinsic curvature, or the way spatial manifolds are embedded in 3+1-space, can also be defined in terms of the projection operator as \( K_{\mu \nu} = -P_\alpha^\mu \nabla_\alpha n_\nu \). A full derivation of the equations of motion can be found in textbooks such as [67] or [68]. The equations of motion are given for \( K_{ij} \) and \( \gamma_{ij} \), typically along with equations...
governing the behavior of the trace of $K$ and determinant of $\gamma$, as

$$\partial_t K_{ij} = \alpha(R_{ij} - 2K_{il}K^l_j + KK_{ij}) - D_iD_j\alpha - 8\pi\alpha(S_{ij} - \frac{1}{2}\gamma_{ij}(S - \rho))$$

$$+ \beta^l \partial_l K_{ij} + K_{il}\partial_j\beta^l + K_{jl}\partial_i\beta^l$$  \hspace{1cm} (2.5)

$$\partial_t \gamma_{ij} = -2\alpha K_{ij} + D_i\beta_j + D_j\beta_i$$  \hspace{1cm} (2.6)

$$\partial_t K = -D_iD^i\alpha + \alpha(K_{ij}K^{ij} + 4\pi(\rho + S)) + \beta^i D_iK$$  \hspace{1cm} (2.7)

$$\partial_t \ln \gamma^{1/2} = -\alpha K + D_i\beta^i,$$  \hspace{1cm} (2.8)

where all quantities are raised, lowered, and derived purely using the spatial metric (ie, the Ricci tensor is computed purely using the given 3-dimensional spatial metric).

The ‘right-hand side’ of the Einstein field equations, or the stress-energy tensor, is also projected onto spatial slices or onto the normal direction using these operators, providing a definition for source terms in the equations of motion:

$$\rho = n_\mu n_\nu T^{\mu\nu}$$

$$S^i = \gamma^i_\mu n_\nu T^{\mu\nu}$$

$$S_{ij} = \gamma_{i\mu} \gamma^i_{j\nu} T^{\mu\nu}$$

$$S = \gamma_{ij} S^{ij}$$  \hspace{1cm} (2.9)

From the existence of a set of evolution equations, the ADM formulation allows the Einstein equations to be posed as an initial-value problem. In this form, the equations can readily be integrated numerically, albeit subject to questions of well-posedness.
and stability, which will be discussed in more detail later.

In order to evolve the spacetime, values of the spatial metric and its time derivative need to be known at some initial time at all locations on an initial spatial hypersurface. However, this initial metric cannot be freely chosen, due to several non-dynamical constraints present in the Einstein field equations. These can be written in terms of \(3 + 1\) variables by contracting the Einstein equations with the normal to the spatial slices. The (contracted) Gauss-Codazzi relations are also needed, given by

\[
P^\alpha_\mu P^\beta_\nu R_{\alpha\beta\mu\nu} = R + K^2 - K_{ij}K^{ij},
\]

(2.10)

From this, the four Hamiltonian and momentum constraint equations arise. These equations can be written entirely using the Ricci curvature of the spatial metric, \(R\), and the projected extrinsic curvature \(K_{ij}\),

\[
2N^\mu N^\nu (G_{\mu\nu} - 8\pi T_{\mu\nu}) \equiv \mathcal{H} = 0 = R + K^2 - K_{ij}K^{ij} - 16\pi \rho
\]

(2.11)

\[
2P^{ij\mu} N^\nu (G_{\mu\nu} - 8\pi T_{\mu\nu}) \equiv \mathcal{M}^i = 0 = D_j (K^{ij} - \gamma^{ij} K) - 8\pi S^i.
\]

(2.12)

These are a set of coupled, nonlinear elliptic partial differential equations, whose solution can be quite difficult to obtain in general. Various methods have been developed in order to solve them numerically as well as analytically in certain symmetric cases. Solutions of these equations that are of interest for cosmology will be discussed further in Chapter 4.

Evaluating the constraint equations and subsequently evolving the spacetime re-
quires computing a number of additional quantities. In particular, Christoffel symbols of the first and second kind, the Ricci tensor, and contractions of these quantities with the spatial metric will all need to be determined:

\[
\Gamma^i_{jk} = \Gamma^l_{ij} \Gamma^{lj}_k \quad (2.13)
\]

\[
\Gamma_{ijk} = \frac{1}{2} (\gamma_{ij,k} + \gamma_{ik,j} - \gamma_{jk,i}) \quad (2.14)
\]

\[
R = \gamma^{ij} R_{ij} \quad (2.15)
\]

In general, 3 + 1 quantities with purely spatial indices are spatial quantities, whose indices are raised and lowered using the 3-metric.

2.1.1 FLRW in 3+1

In the special case of a Friedmann–Lemaître–Robertson–Walker (FLRW) universe, metric quantities can be translated from the typical FLRW notation to the ADM variables. The FLRW metric is given by

\[
\gamma_{ij} = a^2 \delta_{ij} \quad (2.16)
\]

from which we see that \( \gamma = \det \gamma_{ij} = a^6 \). From the equation of motion for the determinant \( \gamma \), we can derive the Friedmann equations. In geodesic slicing (where \( \alpha = 1 \) and \( \beta^i = 0 \)), the evolution equation for \( \gamma \), Eq. 2.8 relates the extrinsic curvature
and Hubble factor $H \equiv \dot{a}/a,$

$$\frac{16\dot{a}a^5}{2} - \frac{d}{dt} = 3H = -K. \quad (2.17)$$

We can use this expression to compare concepts from the full framework of General Relativity - the extrinsic curvature and metric determinant - to quantities in an FLRW universe: $H \sim -\frac{1}{3}K$ and $a \sim \gamma^{1/6}.$

### 2.2 The BSSNOK Formulation

The BSSNOK formulation evolves a set of metric variables related to the ADM variables through a conformal transformation. In terms of the ADM variables, the BSSNOK variables are

$$e^{12\phi} = \det(\gamma_{ij})$$

$$\bar{\gamma}_{ij} = e^{4\phi}\gamma_{ij}$$

$$K = \text{tr} K_{ij}$$

$$\bar{A}_{ij} = e^{-4\phi}K_{ij} - \frac{1}{3}\bar{\gamma}_{ij}K. \quad (2.18)$$

In general, quantities (including covariant derivatives) notated with bars are raised, lowered, or evaluated using the conformal 3-metric, $\bar{\gamma}_{ij}.$ Unbarred quantities such as source terms are raised, lowered, or evaluated using the full (non-conformal) 3-metric. The conformal metric has been chosen to have a unit determinant, $\det \bar{\gamma}_{ij} = 1,$ and
the variable $\bar{A}_{ij}$ is trace-free. The evolution equations for the BSSNOK variables follow directly from substituting these variables in the ADM evolution equations and manipulating the result, producing

$$\partial_t \phi = -\frac{1}{6} \alpha K + \beta^i \partial_i \phi + \frac{1}{6} \partial_i \beta^i ,$$

(2.19)

$$\partial_t \bar{\gamma}_{ij} = -2\alpha \bar{A}_{ij} + \beta^k \partial_k \bar{\gamma}_{ij} + \bar{\gamma}_{ik} \partial_j \beta^k + \bar{\gamma}_{kj} \partial_i \beta^k - \frac{2}{3} \bar{\gamma}_{ij} \partial_k \beta^k ,$$

(2.20)

$$\partial_t K = -\gamma^{ij} D_j D_i \alpha + \alpha (\bar{A}_{ij} \bar{A}^{ij} + \frac{1}{3} K^2) + 4\pi \alpha (\rho + S) + \beta^i \partial_i K ,$$

(2.21)

$$\partial_t \bar{A}_{ij} = e^{-4\phi} (-\partial_i \partial_j \alpha) + \alpha (R_{ij} - 8\pi S_{ij})^T + \alpha (K \bar{A}_{ij} - 2\bar{A}_{il} \bar{A}^l_j)$$

$$+ \beta^k \partial_k \bar{A}_{ij} + \bar{A}_{ik} \partial_j \beta^k + \bar{A}_{kj} \partial_i \beta^k - \frac{2}{3} \bar{A}_{ij} \partial_k \beta^k .$$

(2.22)

The stability properties of the system can be improved by evolving an additional auxiliary variable, $\bar{\Gamma}^i \equiv \bar{\gamma}^{jk} \bar{\Gamma}_{jk}^i$, which is just a contraction of a conformal Christoffel symbol. Evolving this variable circumvents the need to compute mixed derivative terms when computing the Ricci tensor. However, simply writing down an evolution equation for this variable is not sufficient for evolution, as such systems have been shown to exhibit numerical instabilities. An appropriate multiple of the momentum constraint equation is therefore added to this system in order to stabilize it. A deeper discussion of this problem and why this solution helps can be found in, eg, [68].

In order to implement this, the evolution equation for $\bar{\Gamma}^i$ can be written as

$$\partial_t \bar{\Gamma}^i = -2\bar{A}^{ij} \partial_j \alpha + 2\alpha \left( \bar{\Gamma}^i_{jk} \bar{A}^{jk} - \frac{2}{3} \bar{\gamma}^{ij} \partial_j \Delta K - 8\pi \bar{\gamma}^{ij} S_j + 6\bar{A}^{ij} \partial_j \Delta \phi \right)$$

$$+ \beta^j \partial_j \bar{\Gamma}^i - \bar{\gamma}^{ij} \partial_j \beta^i + \frac{2}{3} \bar{\gamma}^{ij} \partial_k \beta^j + \frac{1}{3} \bar{\gamma}^{ij} \partial_k \beta^j + \bar{\gamma}^{ij} \partial_k \beta^j .$$

(2.23)
In terms of this variable, the conformal metric, and the conformal factor, the Ricci tensor can be written as

\[ R_{ij} = \tilde{R}_{ij} + R^\phi_{ij}, \quad (2.24) \]

with

\[
\tilde{R}_{ij} = -\frac{1}{2} \tilde{\gamma}^l m \tilde{\gamma}_{ij,lm} + \tilde{\gamma}_{k(i} \partial_j ) \tilde{\Gamma}^k - \tilde{\Gamma}^l_{ik} \tilde{\Gamma}^k_{jl} \\
- \frac{1}{2} (\tilde{\gamma}_{d,k} \tilde{\gamma}^{kl} + \tilde{\gamma}_{jl,k} \tilde{\gamma}^{kl} - \tilde{\Gamma}^l_{ij,d} ) \quad \text{and} \quad (2.25) \\
R^\phi_{ij} = -2 \left( \partial_i \partial_j \phi - \tilde{\Gamma}^k_{ij} \partial_k \phi + \tilde{\gamma}_{ij} (\tilde{\gamma}^l m \partial_m \partial_\phi - \tilde{\Gamma}^k \partial_k \phi) \right) \\
+ 4 \left( \partial_l \phi \partial_j \phi - \tilde{\gamma}_{ij} \tilde{\gamma}^l m \partial_l \phi \partial_m \phi \right). \quad (2.26)
\]

A number of variants of these expressions exist in the literature, and some numerical comparisons have been made between them \[69\].

### 2.3 Reference Metric Formulation

While the BSSNOK variables are well-suited for stable numerical evolution, directly integrating them can result in truncation errors in regimes where metric fluctuations are small compared to a dominant FLRW behavior of a spacetime, and overwhelm the behavior of the fluctuations. Contrarily, in regimes where fluctuations are not small, error from discretization, or finite-differencing, can dominate. In order to mitigate truncation error and take full advantage of available numerical precision, a known, dominant spacetime contribution can be subtracted from the evolution equations, and later re-introduced when physical metric quantities are needed. This idea has
been explored in situations where the metric is of a known form, in particular when a coordinate system is singular at points. This idea can be employed to more accurately resolve physics in regimes close to cosmological solutions with an FLRW background, as the FLRW metric solution can be subtracted from the BSSNOK equations of motion. The general FLRW solution is written in terms of the BSSNOK variables as

\[
\begin{align*}
\partial_t \phi_{\text{FLRW}} &= -\frac{1}{6} K_{\text{FLRW}} \\
\partial_t K_{\text{FLRW}} &= \frac{1}{3} K_{\text{FLRW}}^2 + \frac{4}{3} \pi (\rho_{\text{FLRW}} + S_{\text{FLRW}}). \tag{2.27}
\end{align*}
\]

Difference variables are defined in terms of this solution as

\[
\begin{align*}
\Delta \phi &\equiv \phi - \phi_{\text{FLRW}}, \\
\Delta K &\equiv K - K_{\text{FLRW}}, \\
\Delta \rho &\equiv \rho - \rho_{\text{FLRW}}, \\
\Delta S &\equiv S - S_{\text{FLRW}}, \\
\Delta \bar{\gamma}_{ij} &\equiv \bar{\gamma}_{ij} - \bar{\delta}_{ij}, \text{ and} \\
\Delta \alpha &\equiv \alpha - \alpha_{\text{FLRW}}. \tag{2.28}
\end{align*}
\]

While the difference variables defined here are well-suited to problems where the solution is close to the FLRW metric, the difference does not need to be small. It is still possible to study strongly gravitating spacetimes, and indeed, the original BSSNOK formulation is recovered when all of the FLRW reference variables are set to zero. In
this system, the FLRW lapse is typically taken to be either unity (geodesic slicing) or \( \alpha_{\text{FLRW}} = e^{2\phi_{\text{FLRW}}} \) in a ‘comoving’ coordinate system where the time coordinate is conformally related to time in geodesic slicing.

Subtracting the evolution equations for the BSSNOK system and the FLRW solution, the evolution equations for the difference variables can be written,

\[
\partial_t \Delta \phi = -\frac{1}{6} (\alpha \Delta K + \Delta \alpha K_{\text{FLRW}}) + \beta^i \partial_i \Delta \phi + \frac{1}{6} \partial_i \beta^i \quad (2.29)
\]
\[
\partial_t \Delta \bar{\gamma}_{ij} = -2\alpha \bar{A}_{ij} + \beta^k \partial_k \Delta \bar{\gamma}_{ij} + \bar{\gamma}_{ik} \partial_j \beta^k + \bar{\gamma}_{kj} \partial_i \beta^k - \frac{2}{3} \bar{\gamma}_{ij} \partial_k \beta^k \quad (2.30)
\]
\[
\partial_t \Delta K = -\gamma^{ij} D_i D_j \Delta \alpha + \alpha \left( \bar{A}_{ij} \bar{A}^{ij} + \frac{1}{3} \Delta K (\Delta K + 2 K_{\text{FLRW}}) \right) + 4\pi (\alpha (\Delta \rho + \Delta S) + \Delta \alpha (\rho_{\text{FLRW}} + S_{\text{FLRW}})) + \beta^i \partial_i \Delta K \quad (2.31)
\]
\[
\partial_t \bar{A}_{ij} = e^{-4\phi} (- (D_i D_j \Delta \alpha) + \alpha (R_{ij} - 8\pi S_{ij}))^{\text{TF}} + \alpha (K \bar{A}_{ij} - 2 \bar{A}_i \bar{A}^j) + \beta^k \partial_k \bar{A}_{ij} + \bar{A}_{ik} \partial_j \beta^k + \bar{A}_{kj} \partial_i \beta^k - \frac{2}{3} \bar{A}_{ij} \partial_k \beta^k. \quad (2.32)
\]

In this system, spatial derivatives should be computed by using the difference variables (as there are no spatial gradients in the FLRW solution), and standard quantities from the BSSNOK formulation can be computed by summing the difference and reference FLRW solution.

As a final note on the equations of motion in strongly gravitating regions, it is possible for the conformal factor \( \phi \) to become divergent. To remedy this, an inverse conformal factor \( \chi = e^{-4\phi} \) has been introduced \[9\]. The equation of motion for \( \chi \) is \[
\partial_t \chi = \frac{2}{3} \chi (\alpha K - \partial_i \beta^i) + \beta^i \partial_i \chi. \quad (2.33)
\]
In terms of reference variables, the conformal factor $\chi$ can be written as $\Delta \chi = \chi - \chi_{\text{FLRW}}$. Subtracting the FLRW equation of motion for $\chi_{\text{FLRW}}$ from the above equation of motion results in an equation for the reference variable,

$$\partial_t \Delta \chi = \frac{2}{3} \chi (\alpha \Delta K + \Delta \alpha K_{\text{FLRW}} - \partial_i \beta^i) + \frac{2}{3} K_{\text{FLRW}} \alpha_{\text{FLRW}} \Delta \chi + \beta^i \partial_i \chi.$$  (2.34)

When using the $\chi$-conformal factor instead of $\phi$, the equations of motion containing factors of $\phi$ can be written in terms of $\chi$ instead.

### 2.4 Algebraic Constraint Enforcement

Several nuances are worth mentioning with regard to computing the evolution of the difference variables. In typical codes solving the BSSNOK system of equations, algebraic constraints are sometimes enforced. These algebraic constraints are notated as

$$G^i \equiv \bar{\Gamma}^i + \partial_j \bar{\gamma}^{ij} = 0$$  (2.35)

$$S \equiv \det \bar{\gamma}_{ij} - 1 = 0$$  (2.36)

$$A \equiv \bar{\gamma}^{ij} \bar{A}_{ij} = 0.$$  (2.37)

When computing these and other quantities, it is important to ensure that no ‘$1+\epsilon-1$’ calculations occur. This may happen, in particular, when computing the inverse metric, normalizing the metric, or ensuring the trace-free variable $\bar{A}_{ij}$ remains so.
Keeping this in mind, components of the inverse metric are computed algebraically, directly from the metric. For the conformal 3-metric with unit determinant, the components of the inverse are (exactly) given by

\[
\begin{align*}
\bar{\gamma}^{11} &= 1 - \Delta \bar{\gamma}^2_{23} + \Delta \bar{\gamma}^{22} + \Delta \bar{\gamma}^{22} \Delta \bar{\gamma}^{33} + \Delta \bar{\gamma}^{33} \\
\bar{\gamma}^{22} &= 1 - \Delta \bar{\gamma}^1_{13} + \Delta \bar{\gamma}^{11} + \Delta \bar{\gamma}^{11} \Delta \bar{\gamma}^{22} + \Delta \bar{\gamma}^{22} \\
\bar{\gamma}^{33} &= 1 - \Delta \bar{\gamma}^1_{12} + \Delta \bar{\gamma}^{11} + \Delta \bar{\gamma}^{11} \Delta \bar{\gamma}^{22} + \Delta \bar{\gamma}^{22} \\
\bar{\gamma}^{12} &= \Delta \bar{\gamma}^{13} \Delta \bar{\gamma}^{23} - \Delta \bar{\gamma}^{33} \Delta \bar{\gamma}^{12} - \Delta \bar{\gamma}^{12} \\
\bar{\gamma}^{13} &= \Delta \bar{\gamma}^{12} \Delta \bar{\gamma}^{23} - \Delta \bar{\gamma}^{22} \Delta \bar{\gamma}^{13} - \Delta \bar{\gamma}^{13} \\
\bar{\gamma}^{23} &= \Delta \bar{\gamma}^{12} \Delta \bar{\gamma}^{13} - \Delta \bar{\gamma}^{11} \Delta \bar{\gamma}^{23} - \Delta \bar{\gamma}^{23}.
\end{align*}
\]

Similarly, enforcing normalization of the conformal 3-metric can involve some subtlety. The determinant of the barred metric should be unity, so that \(\det(\delta_{ij} + \Delta \bar{\gamma}_{ij}) = 1\). In order to prevent any violation of this condition, a rescaling is commonly performed, taking \(\bar{\gamma}_{ij} \rightarrow \bar{\gamma}_{ij} / \det(\bar{\gamma}_{ij})^{1/3}\). In order to perform a similar normalization for the difference variable, this rescaling needs to be manipulated into a suitable form. This can be accomplished by writing the rescaling in terms of difference variables:

\[
\begin{align*}
\delta_{ij} + \Delta \bar{\gamma}_{ij} &\rightarrow (\delta_{ij} + \Delta \bar{\gamma}_{ij}) / \det(\bar{\gamma}_{ij})^{1/3}, \text{ or} \\
\Delta \bar{\gamma}_{ij} &\rightarrow (\delta_{ij} + \Delta \bar{\gamma}_{ij}) / \det(\bar{\gamma}_{ij})^{1/3} - \delta_{ij} \\
&\quad = \frac{\Delta \bar{\gamma}_{ij}}{\det(\bar{\gamma}_{ij})^{1/3}} - \delta_{ij} (1 - \det(\bar{\gamma}_{ij})^{-1/3}).
\end{align*}
\]
The remaining complication lies in accurately computing the right-hand side of this expression for a determinant that will be unity. To accomplish this, the determinant is written out explicitly in terms of components and manipulated into form that can be evaluated by standard functions in the c math library. The procedure starts by explicitly writing the components. Defining

\[
\Delta_{\text{det}} \equiv 1 - \det(\bar{\gamma}_{ij}) = -\Delta \bar{\gamma}_{11} + \Delta \bar{\gamma}_{12}^2 + \Delta \bar{\gamma}_{13}^2 - \Delta \bar{\gamma}_{22} - \Delta \bar{\gamma}_{11} \Delta \bar{\gamma}_{22} + \Delta \bar{\gamma}_{13}^2 \Delta \bar{\gamma}_{22} \\
-2\Delta \bar{\gamma}_{12} \Delta \bar{\gamma}_{13} \Delta \bar{\gamma}_{23} + \Delta \bar{\gamma}_{23}^2 + \Delta \bar{\gamma}_{11} \Delta \bar{\gamma}_{23}^2 - \Delta \bar{\gamma}_{33} - \Delta \bar{\gamma}_{11} \Delta \bar{\gamma}_{33} \\
+ \Delta \bar{\gamma}_{12}^2 \Delta \bar{\gamma}_{33} - \Delta \bar{\gamma}_{22} \Delta \bar{\gamma}_{33} - \Delta \bar{\gamma}_{11} \Delta \bar{\gamma}_{22} \Delta \bar{\gamma}_{33},
\]

(2.40)

this can be used along with the special expm1 function (which accurately computes \(e^x - 1\) for small \(x\)) and the log1p function (which accurately computes \(\log(1 + x)\) for small \(x\)) to compute the difference between the determinant to a power and unity as

\[
1 - \det(\bar{\gamma}_{ij})^{-1/3} = -\text{expm1}(\text{log1p}(-\Delta_{\text{det}})/3).
\]

(2.41)

Ensuring that \(\bar{A}_{ij}\) is trace-free and similarly normalized is simpler, as the naive procedure does not include a \(1 + \epsilon - 1\) calculation. In this case, the rescaling is

\[
\bar{A}_{ij} \to \det(\bar{\gamma})^{-1/3} \left( \bar{A}_{ij} - \frac{1}{3} \bar{A}_{ij} \bar{\gamma}^{ij} \right).
\]

(2.42)

So long as spatial derivatives are taken with respect to the difference variables, the remaining quantities in the evolution equations can largely be computed without
concern for loss of precision. The primary exception is when simultaneously evolving a matter source. In this case, the matter may also be evolved using difference equations. Again, it is important to note that no approximation is being made here. The technique is simply a reformulation of the BSSNOK system of equations into a form where roundoff error due to the dominant FLRW spacetime contribution is mitigated.

2.5 Stability and Constraint Violation Growth

Several ideas have been proposed over the years to further improve stability of the BSSNOK system. A more complete discussion of constraint violation behavior for general 3 + 1 formulations can be found in [72], particularly around Eq. 10.29; and a discussion specifically oriented towards the BSSNOK formulation can be found in [73].

In order to study the behavior of constraint violations in the BSSNOK formulation, it is instructive to write down how the constraint violation variables themselves evolve. The constraints can be broken due to either roundoff error, discretization error (in time or spatial dimensions), or numerical error from initial conditions. When this happens, the constraints will be $C^A = \mathcal{H}, \mathcal{M}^i, \mathcal{G}^i, \mathcal{S}, \mathcal{A} \neq 0$. Assuming none of these will be zero, the equations of motion for a given constraint can be written in terms of other constraints.

For a general 3 + 1 system in which algebraic constraints are obeyed, the evolution of the Hamiltonian and momentum constraint equations can be seen to follow the form of a damped wave equation. Written in geodesic slicing for simplicity, the evolution


\[
\partial_t H = -D_i M^i + 2 K H \tag{2.43}
\]

\[
\partial_t M^i = -D_i H + 2 K^i_j M^j + K M^i. \tag{2.44}
\]

For negative \( K \) (and \( K_{ij} \)) (corresponding to an expanding, cosmological spacetime), the constraints thus obey a damped wave equation, while for positive values the equation can be seen as ‘anti’-damped. In any case, the constraints can be expected to propagate. For simulations with open domains including simulations with damping boundary conditions (common for studies of singularities), it is possible for constraint violation to leave the system of interest entirely. By contrast, for spacetimes with periodic boundary conditions, the constraint violation may not leave the system.

It is possible in principle to increase the amplitude of damping by adding multiples of the constraint violation to the equations of motion. Perhaps the most straightforward modification is adding a multiple of the Hamiltonian constraint to the evolution equation for \( K \) (or \( \Delta K \)),

\[
\partial_t \phi \to \partial_t \phi + \frac{3}{2} \alpha_H H, \tag{2.45}
\]

resulting in a modification of the evolution equation for the Hamiltonian constraint equation,

\[
\partial_t H \supset 2 K H \to \partial_t H \supset 2(1 + \alpha_H) K H. \tag{2.46}
\]

Thus for negative \( K \), the amplitude of constraint damping can be ‘tuned’ by adjusting (increasing) the value of \( \alpha_H \).
A separate analysis can be performed when the algebraic constraints are not satisfied \[73\]. This analysis is substantially more complicated, and will in general depend on precisely which variables are used to compute the Ricci tensor and scalar. To help simplify the procedure, an expansion around a flat spacetime, the Minkowski metric, is performed. In this case, the constraints for the BSSNOK formulation obey the evolution equations

\[
\begin{align*}
\partial_t \mathcal{H} &= -\partial_i \partial^i A \\
\partial_t M^i &= -\partial_j \partial^j G^i - \frac{1}{6} \partial^i \mathcal{H} \\
\partial_t G^i &= 2M^i - \partial^i A \\
\partial_t S &= -2A \\
\partial_t A &= 0 .
\end{align*}
\]

In Fourier space, this set of equations can be cast into a form for easier analysis. The constraints will obey the equation

\[
\partial_t \tilde{C}^A = M^A_B \tilde{C}^B .
\]

The matrix $M^A_B$ describes how the constraints evolve. In general, negative eigenvalues of this matrix correspond to decaying constraints, positive eigenvalues to growing, zero eigenvalues to stationary, and imaginary eigenvalues to propagating constraints. For the ADM formulation, there are two stationary and two propagating constraints (the algebraic constraints do not apply). For the BSSNOK formulation, three are
stationary and six are propagating.

This analysis suggests that the BSSNOK formulation might benefit from additional modifications to the constraint equations in order to obtain decaying constraint behavior. One particularly useful modification to the evolution equation to the trace-free conformal extrinsic curvature $\bar{A}_{ij}$, allows

$$\partial_t \bar{A}_{ij} \rightarrow \partial_t \bar{A}_{ij} + \kappa \alpha \bar{D}_{(i} \mathcal{M}_{j)}.$$  \hspace{1cm} (2.53)

For a value $\kappa > 0$, this modification makes seven of the nine eigenvalues negative. Subsequent studies of this modification have indeed demonstrated diminished constraint violation in evolution of various spacetimes [74].

Several other such constraint-damping systems have been studied in order to perform simulations on longer timescales and more with higher accuracy. Perhaps the most straightforward of these is a modification motivated by the above arguments, first implemented by [75]. The specific modification is the addition of a multiple of the Hamiltonian constraint to the conformal metric, conformal factor, and trace-free conformal extrinsic curvature,

$$\partial_t \phi = \ldots + 0.1c_H \mathcal{H}$$ \hspace{1cm} (2.54)

$$\partial_t \bar{\gamma}_{ij} = \ldots + 0.5c_H \bar{\gamma}_{ij} \mathcal{H}$$ \hspace{1cm} (2.55)

$$\partial_t \bar{A}_{ij} = \ldots - 1.0c_H \bar{A}_{ij} \mathcal{H}$$ \hspace{1cm} (2.56)

for some coefficients $c_H$. The first two of these additions are associated with negative
eigenvalues and thus represent damping terms. The last addition is not motivated by the same argument, but can still be interpreted as the addition of a nonlinear damping term [76].

Two additional significant modifications of the BSSNOK formulation have appeared since the formulation has gained widespread use: the CCZ4 formulation [35,77] (and some variants), and the $C^2$-adjusted formulation [37]. The CCZ4 formulation – and a simpler reduction known as the Z4c formulation [36] – have both demonstrated the ability to damp constraint violations in simulations. The $C^2$-adjusted formulation attempts to drive the system to a constraint surface by adding an effective potential to the equations of motion that penalizes the system for leaving constraint surfaces.

While these constraint systems may lead to longer, more stable evolution, these adjustments may nevertheless pull the solution further away from the correct, physical evolution of the system, and thus may lead to slower convergence to a continuum solution [78]. Thus when using such schemes, it is important to always check for numerical convergence. These ideas will be implemented and explored in more depth in Chapter 5.
Chapter 3

Cosmological Settings

The dynamical behavior of a spacetime is described by the components of the metric, which are determined not only by the physical degrees of freedom inherent in the Einstein field equations, but also by the matter content residing in the spacetime, initial conditions, and choice of gauge. While many forms of matter exist in the Universe, for any preliminary cosmological investigation, approximate, idealized matter sources are commonly used along with practical choices of initial conditions and gauge. This chapter explores these ideas with some generality, then seeks to tailor them to a cosmological setting.

In a general cosmological setting, periodic boundary conditions are often exploited for numerical work. Such boundary conditions are necessary because a finite domain can be resolved in a computational problem; although asymptotically-FLRW boundary conditions or boundary conditions intended to mimic alternative environments could also be used in principle.

Matter components commonly found in a cosmological setting include perfect
fluids, scalar fields, and collisionless matter. Additional sources, including magneto-
hydrodynamical systems and more general fields have been studied, but will not be
considered here.

3.1 Pressureless Fluid Dynamics

A general perfect fluid has a stress-energy tensor of the general form

\[
T^{\mu\nu} = (\rho_0 (1 + W \epsilon) + P) U^{\mu} U^{\nu} + P g^{\mu\nu},
\]

(3.1)

for which \(\rho_0\) is the rest-mass energy density, \(\rho_0 \epsilon W\) any internal (non-rest-mass) energy
density, \(P\) the pressure of the fluid, \(U^{\mu}\) the fluid’s 4-velocity, and \(W = -n_\mu U^\mu\) is the
Lorentz factor. Knowing these quantities, the source terms for the BSSNOK system
(Eq. 2.9) can be constructed.

The challenge then, is to pose the equations of motion for the fluid in a form
suitable for integration in a fully relativistic setting. For fluid evolution, the formation
of shocks – discontinuities in the variables being evolved – is one of the primary
complications. This sharp discontinuity is typically handled in one of two ways:
either a small, artificial numerical viscosity is added to broaden the shock so it can
be resolved by finite differencing methods; or finite-volume schemes are used in which
only the flow of fluid moving across discrete boundaries is tracked. The latter of
these methods is found in many numerical codes, and is accomplished by bringing
the equations of motion for the fluid into a conservative form

\[ D_\mu T^{\mu\nu} = 0 \rightarrow \partial_t U + \partial_i F^i = S \]  

(3.2)

where

\[
U = \begin{pmatrix}
\tilde{D} \\
\tilde{S}_j \\
\tilde{\tau}
\end{pmatrix} \equiv \begin{pmatrix}
\gamma^{1/2} W \rho_0 \\
\gamma^{1/2} \alpha T^0_j \\
\alpha^2 \gamma^{1/2} T^{00} - \tilde{D}
\end{pmatrix}, \\
F^i = \begin{pmatrix}
\tilde{D} v^i \\
\alpha \gamma^{1/2} T^i \\
\alpha^2 \gamma^{1/2} T^{0i} - \tilde{D} v^i
\end{pmatrix},
\]

(3.3)

and

\[
S = \begin{pmatrix}
0 \\
\frac{1}{2} \alpha \gamma^{1/2} T^{\mu\nu} g_{\mu\nu,j} \\
\alpha \gamma^{1/2} \left[ (T^{00} \beta^i \beta^j + 2 T^{0i} \beta^j + T^{ij}) K_{ij} - (T^{00} \beta^i + T^{0i}) \partial_i \alpha \right]
\end{pmatrix}.
\]

(3.4)

In this form, the variables in \( U \) can be seen to obey a conservation law, with \( F^i \) the flux into or out of a region, and \( S \) a source term.

In a cosmological setting, the dominant matter component of the universe has been found to be well-described by a pressureless fluid with no internal energy, so \( P = 0 \) and \( \epsilon = 0 \) [67]. For such a fluid, the solution is described by a series of delta-function density packets traveling through the spacetime. However, this behavior is not evident in the above fluid formulation, because multiple density waves traveling through the same region, or ‘multistreaming’, will not be resolved if only a single velocity is able to be tracked at a given point.
Alternative numerical methods for modeling non-interacting fluid include either integrating the fully relativistic Vlasov equations directly \(^{79}\), or a general relativistic N-body calculation \(^{80, 84}\). The latter of these ideas is commonly implemented in the Newtonian literature, although some direct comparisons between the two approaches \(^{85}\) suggest that a Vlasov approach offers well-defined convergence properties in contrast to the ‘smoothed particle hydrodynamics’ (SPH) N-body approach \(^{86, 87}\). Indeed, the conditions under which SPH schemes converge have only recently been demonstrated \(^{88}\). Nevertheless, Vlasov schemes require substantially more computing resources than an N-body approach, as the entirety of a 6-dimensional phase space needs to be tracked at each point. By contrast, information about particle velocity is only needed at locations where particles exist in the N-body approach.

In a general N-body scheme, particles of a given mass are placed in the spacetime and allowed to evolve. Such particles are taken to interact only gravitationally, and thus follow geodesics. In a suitable 3 + 1 form, the geodesic equation for the particles is (Eq. 1.8)

\[
\begin{align*}
\partial_t U_i & = -\alpha U^0 \partial_i \alpha + U_j \partial_i \beta^j - \frac{1}{2U^0} U_j U_k \partial_i \gamma^{jk} \\
\partial_t x^i & = \frac{1}{U^0} \gamma^{ij} U_j
\end{align*}
\] (3.5) (3.6)
where $U^0 = (1 + \gamma^{ij} U_i U_j)^{1/2}/\alpha$, and source terms for the BSSNOK equations are

\begin{align*}
\rho &= \sum_A m_A n_A W^2 \quad (3.7) \\
S_i &= \sum_A m_A n_A W U_i^A \quad (3.8) \\
S_{ij} &= \sum_A m_A n_A U_i^A U_j^A \quad (3.9) \\
S &= \rho - \sum_A m_A n_A, \quad (3.10)
\end{align*}

with the mass for individual particles $m_A$ and number density $n_A = 1/W\gamma^{1/2}\Delta x^3$ in a space discretized into regions of volume $\Delta x^3$.

While advantageous in its ability to resolve effects in an arbitrary gauge, neither N-body nor Vlasov techniques will be used in this thesis. Another, simpler solution that can be exploited is to study the specific case of a perfect fluid with zero initial coordinate velocity in geodesic slicing. When at rest in this gauge, the equation of motion for the density of a pressureless fluid takes the particularly simple form

$$\partial_t \tilde{D} = 0. \quad (3.11)$$

This conservation law implies that only a single field, $\tilde{D}$, needs to be initialized and does not need to be subsequently evolved. From this variable, the density source term for the BSSNOK equations can be written as $\rho = \rho_0 = \gamma^{-1/2} \alpha \tilde{D}$, and all other source terms will be zero.

As noted earlier, multistreaming cannot be resolved in geodesic slicing using standard fluid techniques. The problem is manifest in this gauge, where the coordinates
can be seen to follow the fluid elements: when fluid elements cross, coordinates will also have to cross. This results in a coordinate singularity causing the simulation to break down. On sufficiently large length scales and sufficiently short time scales, as is the case with results presented in this thesis, this is not an issue. However, at smaller scales when the dynamical timescale is short, simulations can break down very quickly.

A straightforward remedy is to work in a gauge in which such coordinate singularities will not form. Harmonic gauge is commonly chosen in strong gravity regimes, where the lapse function evolution equation is \( \partial_t \alpha = -(K^2 - K^2_0)\alpha \), for some field \( K_0 \) on the initial surface [66]. Importantly, this gauge is also chosen in order to avoid formation of physical singularities, because the timelike distance between spatial slices approaches zero as collapsed regions form.

Harmonic gauge contrasts the gauge used in Newtonian N-body simulations in cosmology, which typically use so-called Newtonian gauge, in which \( \beta^i = 0 \) and \( h_{ij} = 0 \), where \( \gamma_{ij} = (1 - 2\Phi_N)\delta_{ij} + h_{ij} \), for \( \Phi_N \) a scalar function and \( \delta^{ij}h_{ij} = 0 \). While using Newtonian gauge is possible in a linearized perturbative analysis, the gauge imposes more restrictions than are allowed in a fully general relativistic setting, and is therefore considered a ‘restricted gauge’. In this gauge, physical singularities should quickly develop in a universe containing non-interacting matter. However, the explicit formation of singularities is prevented in practice by the introduction of ‘gravitational softening’, or the broadening of the mass distribution of point-like objects. The definition of the gauge is also nonlocal, requiring the solution of an elliptic PDE at every timestep.
3.2 Initial Conditions

For such a pressureless perfect fluid source in geodesic slicing, there are several ways to set initial conditions. The Hamiltonian and momentum constraint equations will need to be solved for a given density $\rho_0$ on the initial surface. The most straightforward solutions can be obtained by considering a conformally flat spacetime, where $\bar{\gamma}_{ij} = \delta_{ij}$ and $\bar{A}_{ij} = 0$, and where the extrinsic curvature is constant. In this case, all terms in the momentum constraint equation are trivially zero. The nonzero terms in the Hamiltonian constraint equation form the system

$$\nabla^2 e^\phi - \frac{e^{5\phi}}{12} K^2 + 2\pi e^{5\phi} \rho = 0. \quad (3.12)$$

In order to see the cases for which this equation has a solution in a periodic spacetime, the integral can be evaluated,

$$\int_V d^3x \left\{ \nabla^2 e^\phi - \frac{e^{5\phi}}{12} K^2 + 2\pi e^{5\phi} \rho \right\} = 0. \quad (3.13)$$

The divergence term will vanish in a periodic spacetime, leaving a constraint on the average value of the extrinsic curvature trace. For the case of a constant extrinsic curvature, the value will be determined by the volume-averaged density

$$K^2 = 24\pi \frac{1}{V} \int_V d^3x \rho = 24\pi \langle \rho \rangle. \quad (3.14)$$
The density can be decomposed into a term obeying this relationship, \( \rho_K = \langle \rho \rangle \), and residual piece, \( \rho_\phi \), so that \( \rho = \rho_K + \rho_\phi \). The residual density will need to satisfy the equation

\[
\nabla^2 e^\phi + 2\pi e^{5\phi} \rho_\phi = 0.
\]

A number of methods exist to solve such nonlinear elliptic equations. Perhaps the most successful of these methods is the ‘multigrid’ scheme, which is an accelerated relaxation technique. However, two more simple methods can be used to construct solutions for this equation.

One method is to specify a conformally related density, \( \bar{\rho} = e^{5\phi} \rho_\phi \), and solve the resulting linear elliptic PDE using a standard Fourier or matrix inversion technique. The more straightforward of these approaches, given widely-available numerical tools, is Fourier inversion of the \( \nabla^2 \) operator. This method proceeds by constructing the Fourier transform of the function \( \bar{\rho} \), performing a sum according to the finite-difference stencil used (described in more detail in Ch. 5), and solving the resulting equations for \( \phi \).

Explicitly performing this calculation is straightforward for the case of a one-dimensional function discretized into \( N \) points using a second-order finite-difference stencil [89]. The inverse Fourier transform of the conformal density, \( \tilde{\bar{\rho}} \), is written as

\[
\tilde{\bar{\rho}}(x) = \sum_{k=0}^{N} \tilde{\bar{\rho}}(k)e^{2\pi ikx/N}.
\]

For a standard second-order finite difference method with derivatives approximated
as
\[ \nabla^2 \psi = \partial_x^2 \psi \simeq \frac{\psi(x - \Delta x) - 2\psi(x) + \psi(x + \Delta x)}{\Delta x^2} , \]  
(3.17)

the corresponding Fourier transform will be
\[
\nabla^2 \tilde{\psi} = \frac{1}{\Delta x^2} \sum_{k=0}^{N} \tilde{\psi}(k) \left( e^{2\pi ik(x-\Delta x)/N} - 2e^{2\pi ikx/N} + e^{2\pi ik(x+\Delta x)/N} \right) \\
= \sum_{k=0}^{N} e^{2\pi ikx/N} \tilde{\psi}(k) \frac{-4}{\Delta x^2} \sin^2\left(\frac{\pi k \Delta x}{N}\right) . \]  
(3.18)

By using the Fourier transform of the conformal density and equating the expressions for each mode (considering Eq. 3.15 in Fourier space) a solution for \( \tilde{\psi} = e^{\phi} \) can be obtained. Finally, computing the inverse Fourier transform yields a solution for \( \phi \),
\[
\psi(x) = \sum_{k=0}^{N} e^{2\pi ikx/N} \tilde{\rho}(k) \frac{\Delta x^2}{\sin^2\left(\frac{\pi k \Delta x}{N}\right)} . \]  
(3.19)

A similar procedure can be followed to construct a full, higher-dimensional solution for arbitrary finite-difference expressions.

The second method for obtaining a solution is substantially more simple: the conformal factor \( \phi \) can be specified, from which the density \( \rho_{\phi} \) can be reconstructed using Eq. 3.15. While both of these methods were attempted and implemented for this work, the latter turns out to be particularly useful due to the accuracy and speed with which solutions can be obtained. However, the Fourier method or the multigrid method may be better-motivated in cases where the density or conformal density is known or given by a particular model.
In the case of late-universe cosmology, the power spectrum of the density fluctuations can be analytically approximated on a spatial hypersurface using a perturbative analysis, and given a number of assumptions \cite{15}. This power spectrum scales in conformal Newtonian gauge as \( P_k \sim k^1 \) at large scales (small \( k \)), and as \( k^{-3} \) at small scales (large \( k \)).

The peak scale on a slice corresponding to ‘today’ is at roughly \( k_* \sim 350 h^{-1} \) Mpc. This is different than the ‘dimensionless power spectrum’, \( \Delta_k \sim k^3 P_k \), sometimes encountered in the literature. Taking this to be a rough approximation for the power spectrum of the conformal density in geodesic slicing allows a phenomenological form for the power spectrum that agrees with the power-law scaling to be written as

\[
P_{\bar{\rho}}^k = P^*_4 \frac{4}{3} \frac{k}{k_*} \frac{k}{k_*}^{4/3},
\]

(3.20)

with \( P_* \) the (maximum) amplitude at \( k_* \). A Gaussian-random realization of this power spectrum can then be created.

An initial field configuration can be chosen for \( \phi \) (or \( \psi = e^{\phi} \)) rather than \( \rho_\phi \) by choosing a spectrum appropriately. The power spectrum scales as \( P^\phi_k \sim \langle \psi \psi \rangle \sim \langle (\bar{\rho}/k^2)(\bar{\rho}/k^2) \rangle \), so that \( P^\phi_k = k^{-4} P^\bar{\rho}_k \). Thus in practice, the conformal factor can be initialized with this power spectrum, and density subsequently computed algebraically with no Fourier analysis needed.
Chapter 4

Optics in Numerical Relativity

The evolution equations presented in Chapter 2 describe the evolution of the metric, a tensor whose values depend on the choice of coordinate system. Using this metric, 3-scalar quantities describing properties of the spacetime can be computed. These include the determinant of the 3-metric, which corresponds to the 3-volume on a spatial slice, and the trace of the extrinsic curvature $K$, which is related to the rate of expansion of this volume. Unfortunately, the values of these quantities still depend on the particular way in which the spacetime has been foliated into spatial slices. In other words, these properties depend on the shape or position of the spatial slices in the 4-dimensional spacetime. Thus, the values of metric components and their time-derivatives will not necessarily be indicative of the behavior of measurable quantities in a spacetime. Questions about physical properties of the spacetime are therefore best posed in terms of measurable quantities.

At a basic level, cosmological observations are made by measuring the energy
deposited by particles (typically photons) on a receiver\(^1\). The behavior of beams of light traveling through a spacetime, known as geometric optics, will thus form a basis on which observational questions can be addressed.

The remainder of this chapter is devoted to describing the formalism of geometric optics in a fully relativistic spacetime. The formalism is then written in terms of standard 3 + 1 quantities, ensuring suitability for numerical integration – something that has not yet been done in existing literature.

### 4.1 Integration of geodesics

In this section, the equations governing the motion of particles following geodesics are presented, following the notation and procedure of \[92\]. Although null geodesics will be of particular interest, illustrated in Figure 4.1, the equations presented here can be applied to massive particles as well.

The equations describing evolution along a geodesic are typically parametrized by an affine variable. These equations will need to be re-parametrized in terms of the coordinate time \(t\) and variables from a 3+1 split. In terms of such an affine parameter \(\lambda\), the 4-momentum vector \(p^\mu\) for a particle following a geodesic is defined by

\[
p^\mu = \frac{dX^\mu}{d\lambda} .
\] (4.1)

\(^1\)Some measurements make use of charged particle spectrometers or detectors, and the recent direct detections of gravitational waves \[90,91\] has provided another unique observational tool.
Figure 4.1: An illustration of integrating geodesics through a spacetime with density fluctuations. Shades of lighter gray represent denser regions of space, and darker colors represent less dense regions. In a time-reversed sense, light rays (yellow) originate from an observer located in the volume and propagate outward along null geodesics.

A similar quantity can be defined with respect to coordinate time,

\[
\frac{dX^\mu}{dt} = q^\mu
\]  

(4.2)

so that

\[
\frac{1}{p^0}p^\mu = q^\mu.
\]  

(4.3)

The energy of the particle projected onto the spatial slice, \( E \), can also be written in terms of the normal and 4-momentum, \( E = -n_\mu p^\mu \). The quantity \( p^0 \) can be related to \( E \) by noting that \( n_\mu dX^\mu = n_\mu p^\mu d\lambda \), a statement that reduces to \( E/\alpha = p^0 \).
The 4-momentum $p^\mu$ can then be decomposed into a piece parallel to the normal, $p_\parallel \propto n^\mu$, and a tangent piece, $p_\perp$,

\[
\begin{align*}
p_\parallel^\mu &= p^\mu - En^\mu \equiv EV^\mu \quad \text{(4.4)} \\
p_\perp^\mu &= p^\mu - p_\parallel^\mu = En^\mu. \quad \text{(4.5)}
\end{align*}
\]

The 4-momentum can be written in terms of these components, $p^\mu = E(n^\mu + V^\mu)$. The velocity 3-vector $V^i$ represents the velocity of a particle as seen by a normal observer. Because $n_\mu V^\mu = 0$, the time component of the velocity vector should be zero, or $V^\mu = (0, V^i)$. At this point the components of the coordinate 4-momentum vector can be written as $q^\mu = \alpha (n^\mu + V^\mu) = (1, \alpha V^i - \beta^i)$.

Evolution equations for the $3+1$ quantities $E$ and $V^i$ can be found from the geodesic equation. As seen in Eq. 1.9, the geodesic equation is

\[
\frac{d^2 X^\mu}{d\lambda^2} = -\Gamma^\mu_{\alpha\beta} \frac{dX^\alpha}{d\lambda} \frac{dX^\beta}{d\lambda}
\]

(4.6)

for the position of a particle $X^\mu$ along a path parametrized by $\lambda$. While the equation in this form is not well-suited to numerical integration, it can be re-cast in terms of a coordinate time $t$ using the chain rule,

\[
\frac{d^2 X^\mu}{dt^2} = \frac{d}{dt} \left( \frac{d\lambda}{dt} \frac{dX^\mu}{d\lambda} \right) = -\Gamma^\mu_{\alpha\beta} \frac{dX^\alpha}{dt} \frac{dX^\beta}{dt} + \Gamma^\mu_{\alpha\beta} \frac{dX^\alpha}{dt} \frac{dX^\beta}{dt} \frac{dX^\mu}{dt}.
\]

(4.7)
When $\mu = 0$, both sides of this equation vanish identically. An evolution equation for $p^0$ can instead be written as

$$\frac{d}{dt}p^0 = \frac{1}{p^0} \frac{d}{d\lambda} p^0 = -\frac{1}{p^0} \Gamma^0_{\alpha\beta} p^\alpha p^\beta ,$$

(4.8)

from which an evolution equation for $E$ can be derived

$$\frac{d}{dt}E = \alpha \frac{d}{dt} p^0 + p^0 \frac{d}{dt} \alpha$$

$$= \alpha \frac{d}{dt} p^0 + p^0 \partial_t \alpha + \frac{dX_i}{dt} \partial_i \alpha$$

$$= E \left( -\Gamma^0_{\alpha\beta} q^\alpha q^\beta + \partial_t \ln \alpha + q^i \partial_i \alpha \right) .$$

(4.11)

In order to express this system in terms of BSSNOK or ADM variables, the Christoffel symbols need to be written in terms of the 3 + 1 metric components. The relevant Christoffel symbols are

$$\Gamma^0_{ij} = -\frac{1}{\alpha} K_{ij}$$

(4.12)

$$\Gamma^0_{i0} = \Gamma^0_{0i} = \frac{1}{\alpha} \left( \partial_i \alpha - \beta^j K_{ij} \right)$$

(4.13)

$$\Gamma^0_{00} = \partial_t \ln \alpha + \beta^i \Gamma^0_{0i}$$

$$= \partial_t \ln \alpha + \frac{1}{\alpha} \left( \beta^i \partial_i \alpha - \beta^i \beta^j K_{ij} \right) .$$

(4.14)

(4.15)

Manipulating into a more suitable form, the evolution equations for $E$ and $V^i$ reduce
\[
\frac{dX^i}{dt} = \alpha V^i - \beta^i \\
\frac{dV^i}{dt} = \alpha V^j \left( V^i \partial_j \ln \alpha - K^i_{jk} V^k V^i + 2K^i_j \right) \\
\quad - \left( \Gamma^i_{jk} V^k \right) - \gamma^{ij} \partial_j \alpha - V^j \partial_j \beta^i \\
\frac{dE}{dt} = E \left( \alpha K_{ij} V^i V^j - V^j \partial_j \alpha \right).
\]

\[ (4.16) \]
\[ (4.17) \]
\[ (4.18) \]

### 4.2 Optical Scalar Equations

Computing cosmological observables, such as angular diameter distances, requires the area of light beams to be tracked along geodesics. The formalism of geometric optics provides the necessary framework. While the only approximation made in this formalism is that the beam size is small (infinitesimal), it also requires that additional (non-gravitational) physics does not directly affect areas of beams as they propagate, and that general relativity itself is valid. The small beam approximation should therefore provide a very good approximation for point-like sources such as supernovae, but not necessarily for beams with a large angular extent, such as measurements of baryon acoustic oscillations or measurements of fluctuations in the cosmic microwave background.

The equations describing the evolution of the beam area begin with the optical
focusing equations [93].

\[
\frac{d}{d\lambda} \theta + \theta^2 + |\sigma|^2 = \mathcal{R}
\]

\[
\frac{d}{d\lambda} \sigma + 2\theta \sigma = \mathcal{W}.
\]  

(4.19)

Here, \( \theta = \frac{1}{2A} \frac{dA}{d\lambda} \) describes the expansion rate of the beam area \( A \) (which is not an angle). In this thesis, the square root of the beam area, \( \ell = \sqrt{A} \), will be tracked. The quantity \( \sigma \) is a complex scalar, which roughly describes the rate of ‘shearing’ (expansion along one axis and compression along another) of a light beam. The Weyl and Ricci optical scalars, \( \mathcal{W} \) and \( \mathcal{R} \) respectively, are given by

\[
\mathcal{W} = -\frac{1}{2} C_{\mu \nu \rho \sigma} (s_1^\mu - is_2^\mu) p^\nu (s_1^\sigma - is_2^\sigma)
\]  

(4.20)

\[
\mathcal{R} = -4\pi T_{\mu \nu} p^\mu p^\nu = -\frac{1}{2} R_{\mu \nu} p^\mu p^\nu
\]  

(4.21)

for screen vectors \( s_1^\mu, s_2^\mu \), and Weyl tensor \( C_{\mu \nu \rho \sigma} \). The Weyl and Ricci scalars respectively source beam shearing due to stretching of a spacetime, and focusing of a beam due to matter content present in the universe intercepted by the beam. Here, the Weyl scalar is analogous to the Weyl scalars in the Newman-Penrose formalism for identifying gravitational radiation [94]. However, the vectors used for computing the Weyl scalar are comprised of a single null vector \( p^\mu \) and the screen vectors, rather than a null tetrad.

The screen vectors obey various orthogonality relationships: \( g_{\mu \nu} s_N^\nu p^\mu = 0 \) (normal to the photon 4-vector), \( g_{\mu \nu} s_N^\nu (q^\mu - U^\mu) \equiv g_{\mu \nu} s_N^\nu d^\mu = 0 \) (normal to the “direction
of observation” $d^\mu$ and thus observer 4-velocity $U^\mu$, and $g_{\mu\nu}s_1^\mu s_2^\nu = 0$ and $g_{\mu\nu}s_1^\mu s_1^\nu = g_{\mu\nu}s_2^\mu s_2^\nu = 1$ (orthonormality of $s_1^\mu$ and $s_2^\mu$). Additionally, they obey a partial parallel transport equation \[95\],

$$S_\nu^\mu \frac{D s_\nu^\nu}{d\lambda} = 0$$

(4.22)

for a screen projection operator $S^\mu{}^\nu = g^\mu{}^\nu + U^\mu U^\nu - d^\mu d^\nu$ and covariant derivative along the beam’s path, $\frac{D}{d\lambda} = k^\mu D_\mu$. Written in 3+1 form in synchronous gauge, the evolution equations for the screen vectors become

$$\frac{d}{dt} s_i^A = s_i^A V^i \left( \gamma_{jk} \frac{d}{dt} V^k - 3V^k K_{jk} + V_l V^k \Gamma_{lkj} \right)$$

$$- \Gamma_{kl} V^k s_l^A + \gamma^{ij} K_{jk} s_k^A ,$$

(4.23)

with the term including the time derivative of $V^k$ determined by the left-hand side of Eq. 4.17. The beam area will be invariant under rotations of the screen vectors in screen space, though not invariant under a time-dependent rotation. Thus one valuable code test is to vary the initial screen vectors, and verify that there is no resulting change in the computed optical scalars.

Of note, photon polarization vectors obey an almost identical set of equations, which may provide a direct method for computing gravitational effects on polarization. The major difference between the evolution of screen and polarization vectors is only that normalization is enforced for the screen vectors.

In addition to rewriting the optical scalar variable $\theta$ in terms of $\ell$, another variable can be defined that roughly corresponds to the root of the solid angle subtended by
the beam, \( \varphi = d\ell/d\lambda \). When a beam has reached an observer, the angle subtended will be \( d\ell_{\text{obs}}/d\lambda = \sqrt{\Omega_{\text{obs}}} \), with \( \Omega_{\text{obs}} \) the solid angle subtended by the beam. The real and complex pieces of \( \sigma \) will also need to be evolved using evolution equations expressed in terms of coordinate time \( t \). In order to simplify the equations of motion for \( \sigma \), the evolution equations are written in terms of \( \bar{\sigma} = \ell^2 \sigma \). The resulting evolution equations for tracking the beam area and shape are thus:

\[
\begin{align*}
\frac{p^0}{dt} \varphi &= \ell \left( \mathcal{R} - \sigma^2_R - \sigma^2_I \right) \quad (4.24) \\
\frac{p^0}{dt} \ell &= \varphi \quad (4.25) \\
\frac{p^0}{dt} \bar{\sigma}_R &= \ell^2 \Re[\mathcal{W}] \quad (4.26) \\
\frac{p^0}{dt} \bar{\sigma}_I &= \ell^2 \Im[\mathcal{W}] \quad (4.27)
\end{align*}
\]

with the real and imaginary pieces of the Weyl scalar given by

\[
\begin{align*}
\Re[\mathcal{W}] &= -\frac{1}{2} C_{\mu\nu\rho\sigma} (s^\mu_1 s^\sigma_1 - s^\mu_2 s^\sigma_2) p^\nu p^\rho \quad (4.28) \\
\Im[\mathcal{W}] &= C_{\mu\nu\sigma} s^\mu_1 p^\nu s^\sigma_2 . \quad (4.29)
\end{align*}
\]

These equations are subject to boundary conditions at a point of observation, namely that the beam area has converged so \( \ell(t_{\text{obs}}) = 0 \), that an observer views the beam as subtending some solid angle, \( \varphi(t_{\text{obs}}) = \sqrt{\Omega_{\text{obs}}} \), and that the shear rate is \( \sigma = \bar{\sigma} = 0 \).
4.3 Calculation of the Weyl Scalar in Synchronous Gauge

Calculating the components of the Weyl tensor represents the dominant computational expense when integrating the optical scalar equations through an arbitrary spacetime. Computing the contraction of the Weyl tensor with the screen and momentum vectors is most straightforward in synchronous gauge, where $\alpha = 1$ and $\beta^i = 0$. In principle, only ten independent components of the Weyl tensor need to be calculated. However, the calculation can be written purely in terms of the Riemann tensor, whose components are somewhat less complex to compute. This is taken advantage of here, although 21 independent components of the Riemann tensor will need to be computed. The Weyl scalar can be written in terms of the Riemann tensor and its contractions as

\[
W = -\frac{1}{2} \left( R_{\mu\nu\rho\sigma} - \frac{2}{n-2} (g_{\mu[\rho} R_{\sigma]\nu} - g_{\nu[\rho} R_{\sigma]\mu}) \right) \left( s^\mu_1 - is^\mu_2 \right) p^\nu p^\rho \left( s^\sigma_1 - is^\sigma_2 \right) + \frac{2}{(n-1)(n-2)} \left( R g_{\mu[\rho} g_{\sigma]\nu} \right) \left( s^\mu_1 - is^\mu_2 \right) p^\nu p^\rho \left( s^\sigma_1 - is^\sigma_2 \right), \tag{4.30}
\]

where square brackets indicate antisymmetrization, and the last line follows from orthogonality of various vectors.

In order to convert this expression to a usable form, the Riemann tensor will need to be written in terms of 3 + 1 variables. The nonzero Christoffel symbols in

\[
\]
synchronous gauge are written as

\[ \Gamma^i_{j0} = \Gamma^i_{0j} = -K^i_j \quad (4.32) \]
\[ \Gamma^i_{0j} = -K_{ij} \quad (4.33) \]
\[ \Gamma^i_{jk} = (3)\Gamma^i_{jk} \quad (4.34) \]

The components of the Riemann tensor in terms of 3+1 quantities follow from this,

\[ ^{(4)}R_{ilmj} = \frac{1}{2} (\gamma_{ij,lm} - \gamma_{jl,im} - \gamma_{im,lj} + \gamma_{ml,ij}) + \Gamma_{qij} \Gamma_{qlm} - \Gamma_{qim} \Gamma_{qjl} - K_{im} K_{jl} + K_{ij} K_{ml} \quad (4.35) \]
\[ ^{(4)}R_{i0mj} = \partial_j K_{im} - \partial_m K_{ij} + (\gamma_{qi,m} + \Gamma_{imq}) K^q_j - (\gamma_{qi,j} + \Gamma_{ijq}) K^q_m \]
\[ ^{(4)}R_{i00j} = -^{(3)}R_{ij} - K K_{ij} + K^l_i K_{lj} + 8\pi \left( S_{ij} - \frac{1}{2} \gamma_{ij} (S - \rho) \right) \quad (4.35) \]

The Weyl scalar can now be re-expressed so that a minimal number of terms are computed. A naive estimate suggests that \( 4 \cdot 4 \cdot 4 \cdot 4 = 256 \) terms arise after summing the original expression

\[ R_{\alpha\mu\nu\beta} s^\alpha_A k^\mu k^\nu s^\beta_B , \quad (4.36) \]

for \( A, B \in \{1, 2\} \). To reduce the number of terms, the index combination \( \alpha, \mu \equiv A \) can be written as a single index running over all combinations of \( \alpha \) and \( \mu \), and the
substitution $s_A^\alpha k^\mu \equiv \zeta^A_\alpha$ can be applied to give

\[
W \supset -\frac{1}{2} R_{\alpha \mu \nu \beta} s_A^\alpha k^\mu s_B^\beta \\
\equiv \frac{1}{2} R_{AB} s_A^A s_B^B \\
\equiv W^\Sigma_{AB}.
\] (4.37, 4.38, 4.39)

Because the Weyl scalar is antisymmetric in indices $\alpha$ and $\mu$, the indices $A$, $B$ need not run over all values, but only

\[A, B \in \{01, 02, 03, 10, 12, 13, 20, 21, 23, 30, 31, 32\}.\] (4.40)

However, the antisymmetry allows for further simplification. Denoting the canonical ordering of elements $A_c \in \{01, 02, 03, 12, 13, 23\}$ and reversed $A_r \in \{10, 20, 30, 21, 31, 32\}$, so $A \in A_c \cup A_r$,

\[
R_{AB} s_A^A s_B^B = R_{A_c B} s_B^B \left( \zeta^A_\alpha - \zeta^A_\alpha \right) \\
\equiv R_{A_c B} s_B^B \left( 2\zeta^\alpha_{\{A_c\}} \right)
\] (4.41, 4.42)

and similarly for $B$, so

\[
R_{AB} s_A^A s_B^B = 4R_{A_c B_c} s_A^A s_B^B. \\
\] (4.43)

Because $A_c$ runs over six terms, and because $R_{AB}$ is symmetric, only 21 total components of $R_{AB}$ need to be calculated in order to evaluate the sum, along with
the six components in each of $\varsigma_A^{[Ac]}$ and $\varsigma_B^{[Bc]}$. The six $\varsigma_A^{[Ac]}$ are

$$
\varsigma_A^{[01]} = -\frac{1}{2}s_A^1 p^0 \quad \varsigma_A^{[12]} = \frac{1}{2} (s_A^1 p^2 - s_A^2 p^1) \\
\varsigma_A^{[02]} = -\frac{1}{2}s_A^2 p^0 \quad \varsigma_A^{[13]} = \frac{1}{2} (s_A^1 p^3 - s_A^3 p^1) \\
\varsigma_A^{[03]} = -\frac{1}{2}s_A^3 p^0 \quad \varsigma_A^{[23]} = \frac{1}{2} (s_A^2 p^3 - s_A^3 p^2) ,
$$

(4.44)

and can be similarly computed for $\varsigma_B^{[Bc]}$. The vectors $s^\mu$ can be freely chosen so long as only the beam area and opening angle are of interest, and they are orthogonal to $p^\mu$ and the observer’s line of sight, $V_i$. The sum should then contain $6 \cdot 6 = 36$ terms,

$$
\frac{1}{2} \mathcal{W}^{\Sigma}_{AB} = \sum_{A_c,B_c \in \{01,02,03,12,13,23\}} R_{A_cB_c} \varsigma_A^{[Ac]} \varsigma_B^{[Bc]} ,
$$

(4.45)

This includes the 21 unique components of the Riemann tensor that can be evaluated using Eq.4.35. From this, Equation 4.45 can then be used to calculate the source terms for the optical scalar equations,

$$
\Re[\mathcal{W}] = \frac{1}{2} (\mathcal{W}^{\Sigma}_{11} - \mathcal{W}^{\Sigma}_{22}) \\
\Im[\mathcal{W}] = -\mathcal{W}^{\Sigma}_{12} .
$$

(4.46)

(4.47)

While computationally straightforward, the above calculations have been performed in synchronous gauge. However, more general procedures for computing the Weyl tensor have been developed. One notable method is to decompose the Weyl tensor into trace-free, symmetric ‘electric’ and ‘magnetic’ tensors [68], which can subsequently be used to compute the Weyl optical scalar.
4.4 Optics in an FLRW cosmology

The FLRW metric in synchronous gauge is given by

\[
\gamma_{ij} = a^2(t)\delta_{ij} \quad (4.48)
\]

\[
K_{ij} = -\dot{a}a\delta_{ij} = -H\gamma_{ij} \quad (4.49)
\]

where \(H = \dot{a}/a\). For this metric, the photon energy scales as \(E \sim 1/a\), with

\[
\frac{1}{E} \frac{dE}{dt} = -\frac{1}{a} \frac{da}{dt}, \text{ or} \quad (4.50)
\]

\[
\frac{E(t_1)}{E(t_2)} = \frac{a(t_2)}{a(t_1)} \quad (4.51)
\]

at times \(t_1\) and \(t_2\). The velocity evolves similarly as

\[
\frac{V^i(t_1)}{V^i(t_2)} = \frac{a(t_2)}{a(t_1)} \quad . \quad (4.52)
\]

A formula for computing angular diameter distances can be derived by using the prescription from Section 4.2. Although there are certainly more elegant ways to compute angular diameter distances in an FLRW spacetime, an analogous procedure can be applied in more general spacetimes. The derivation begins by noting that the non-zero Christoffel symbols for the FLRW metric are

\[
\Gamma^0_{ij} = -K_{ij} = \dot{a}a\gamma_{ij} \quad (4.53)
\]

\[
\Gamma^i_{j0} = -K^i_j = H\delta^i_j, \quad (4.54)
\]
with the (relevant) nonzero Riemann tensor components given by

\begin{align}
^{(4)}R_{ilmj} &= H^2 a^4 \delta_{im} \delta_{jl} \\
^{(4)}R_{100j} \equiv \omega=0 &= -a\ddot{a} \delta_{ij} .
\end{align}

Without loss of generality, the behavior of a photon traveling in the $z$-direction can be studied, with $p^\mu = E (1, 0, 0, 1)$, and screen vectors $\hat{x}$ and $\hat{y}$. The non-zero $\varsigma_A$ are then

\begin{align}
\varsigma^{[01]}_1 &= -\frac{1}{2} E \\
\varsigma^{[02]}_2 &= -\frac{1}{2} E \\
\varsigma^{[13]}_1 &= \frac{1}{2} E \\
\varsigma^{[23]}_2 &= \frac{1}{2} E \tag{4.57}
\end{align}

from which $W^{\Sigma}_{11}$ can be determined

\begin{align}
W^{\Sigma}_{11} = W^{\Sigma}_{22} &= -4 \left( -R_{1001} \varsigma^{[01]}_A \varsigma^{[01]}_B \\
&+ R_{1313} \varsigma^{[13]}_A \varsigma^{[13]}_B \right) \\
&= -E^2 a \left( \dddot{a} + a\dot{a}^2 \right) , \tag{4.58}
\end{align}

with $W^{\Sigma}_{12} = 0$. As the above terms cancel, there should be no contribution from the Weyl scalar. Although this has been calculated explicitly here, it would be sufficient to simply note that the Weyl tensor is zero for conformally flat spacetimes, and therefore the Weyl optical scalar must be zero.
The Ricci scalar is then given by

\[ R = -4\pi T_{\mu\nu}p^\mu p^\nu \]  
\[ = -\frac{3}{2}H^2E^2. \]

For a matter-dominated FLRW solution, \( a(t) = \left(\frac{t}{t_0}\right)^{2/3} \) and \( H = \frac{2}{3} \frac{1}{t} \). The remaining non-trivial evolution equations are

\[ \frac{d}{dt}\varphi = -\frac{3}{2}\ell H^2E = -\frac{2}{3}E_0t_0^{2/3}t^{-8/3}\ell \]
\[ \frac{d}{dt}\ell = \frac{1}{E}\varphi = t_0^{-2/3}\ell^{2/3}. \]

Given initial conditions \( \ell(t_0) = 0 \) and \( \varphi(t_0) = \sqrt{\Omega_0} \), this equation is solved by

\[ \varphi(t) = \frac{\sqrt{\Omega_0}}{t}t_0^{2/3}\left(3t^{1/3} - 2t_0^{1/3}\right) \]
\[ \ell(t) = 3\sqrt{\Omega_0}t_0^{2/3}\left(t^{1/3} - t_0^{1/3}\right), \]

from which the angular diameter distance, \( D_A(t_{\text{obs}}) = \ell(t_{\text{em}})/\sqrt{\Omega_{\text{obs}}} \), can be deduced. This result is then used analogously to with the ‘usual’ calculation of angular diameter distances,

\[ D_A(t_{\text{em}}, t_{\text{obs}}) = 3t_{\text{em}}^{2/3}\left(t_{\text{obs}}^{1/3} - t_{\text{em}}^{1/3}\right). \]
Chapter 5

Numerical Methods

This chapter contains a description of the Cosmological General Relativistic And Perfect fluid Hydrodynamics Code, or CosmoGRAPH code, the main tool developed for this thesis. CosmoGRAPH is a unique grid-based code that implements numerical solvers for many of the equations presented in the previous chapters. Generally speaking, numerical techniques provide a complementary approach to analytic techniques when seeking solutions to physical problems. The power of analytic approaches typically lies in their ability to quickly determine solutions for a wide range of parameters. However, obtaining analytic solutions often requires making approximations, reductions based on arguments of symmetry, or other simplifying assumptions; and in the end answers typically require numerical evaluation of special functions regardless. Numerical techniques are complementary to analytic techniques in that they can readily obtain solutions for highly asymmetric, complicated systems, but may struggle to fully explore solutions for models with large parameter spaces.

Analytic solutions of the Einstein field equations are particularly difficult to obtain
due to the complexity of the equations, especially in a cosmological setting where a
variety of matter sources may be of interest. CosmoGRAPh was created to explore
the effectiveness and applicability of the techniques developed for modeling strongly
gravitating compact objects to cosmology. The intent of this code is not to be compet-
itive with the highest-performing codes, either from numerical relativity or cosmology,
although such an achievement could perhaps be realized with (significant) additional
time and effort. Rather, the code has been used to explore the aforementioned refer-
ence formulation of the BSSNOK equations, and the usefulness of numerical relativity
for examining the optical properties of spacetimes in a fully relativistic, cosmological
setting.

CosmoGRAPh is a modern c++ code, which uses features from the c++11 stan-
dard. It makes use of several libraries, including fftw3 for computing Fourier trans-
forms, hdf5 for efficiently reading and writing large amounts of data, and libz for
writing compressed ascii data. The OpenMP API is used to parallelize the code, and
exploratory work using MPI and OpenACC directives has been done. The project is
built using cmake, and typically compiled with the GNU compiler g++, version 4.7
or later as it supports c++11 features. It has also been demonstrated to work with
the Intel compiler icpc, and LLVM compiler clang++. At the time of this writing,
CosmoGRAPh is open source, contains documentation that can be generated using
doxygen, and is actively developed by the cwru-pat group on github[1][2]

[1] The code repository may be found at https://github.com/cwru-pat/cosmograph
[2] A website and code documentation may be found at https://cwru-pat.github.io/cosmograph
5.1 Project Structure

Because CosmoGRAPH is written in C++, an object-oriented language, the program is divided into various classes, containing conceptually distinct components.

A polymorphic base CosmoSim class contains common functionality intended to be inherited by derived classes for simulations of spacetimes with additional components. Simulations are declared as CosmoSim types, then initialized as derived classes based on a simulation type specified by a user. Figure 5.1 shows an inheritance diagram depicting relationships between derived types.

![Inheritance Diagram](image)

Figure 5.1: This inheritance diagram shows the derived classes that inherit the CosmoSim class. Additional diagrams are generated as part of doxygen documentation using the ‘dot’ tool from the graphviz graph drawing toolkit.

While the overall flow of the program is determined by these individual simulation classes, the simulation classes contain different components (also classes) as members depending on both the matter source being evolved and auxiliary calculations needed. These components include a class for solving the reference formulation of the BSS-NOK system; matter sources including a pressureless fluid source in synchronous gauge (dust), scalar field, and a developmental collisionless N-body system; and a

---

3Note that future development may render the description provided here obsolete.
raytracing component for performing optical calculations. A collaboration diagram showing the components used in the CosmoSim class, as well as additional members of this class, can be found in Fig. 5.2. The BSSN class in this diagram provides the functionality for evolving the reference BSSNOK system. Indeed, only a small number of control functions need to be added to this class in order to evolve a vacuum spacetime (implemented in the VacuumSim class).

5.1.1 Numerical Integration

As a set of coupled partial differential equations, the Einstein equations along with matter sources can be integrated using any number of explicit or implicit methods. The explicit 4th-order Runge-Kutta (RK4) method is commonly found in the literature for PDE integration, and often used by codes implementing the BSSNOK formulation. While lacking the stability inherent in many implicit methods, the RK4 method has been demonstrated to perform well when evolving the BSSNOK system and does not require the non-local calculations used in implicit methods.

The basic integration procedure is performed in an RK4Register class. This class contains four CosmoArray classes, which both store grid data as an array, and contain some metadata about the array. Given some differential and/or algebraic operator $D$, the goal of this class is to solve an equation of the form

$$\frac{d}{dt} y(x,t) = D[y(x,t)]$$

(5.1)

for $y$ at a future time $y(x,t = t_0 + \Delta t)$ given a known $y(x,t = t_0)$. For the case
Figure 5.2: A collaboration diagram showing the hierarchy of class members for the CosmoSim class. Diagrams are generated as part of doxygen documentation using the ‘dot’ tool from the graphviz graph drawing toolkit, and can be found in the code documentation.
of multiple, coupled equations, \( y \) represents a set of fields, \( f \) a set of functions, and \( D \) an operator that can include spatial derivatives of the fields. Numerically, given some initial data \( y_p \) (from the previous step), the RK4 calculation is performed using additional arrays \( y_a \) (data actively being used for calculations), \( y_c \) (storage for any intermediate computation), and \( y_f \) (the final result from the RK4 step). The integration step is then performed as described in Fig. 5.3. This routine coincides with other presentations of the RK4 method, and is accurate to \( \mathcal{O}(\Delta t^5) \). Given a total integration time of \( T \) divided into substeps of size \( \Delta t \), error will accumulate at each step; thus the total accumulated error is \( \mathcal{O}(\Delta t^4) \). One advantage of this implementation is that it allows the majority of the integration routine to be handled by a separate class. An \texttt{RK4Register} class has been implemented in order to perform the integration in \textsc{CosmoGraph}, while evaluation of the right-hand side of Eq. 5.1 is generally performed in component classes. Further details, including a description of interaction between components, is made available in the code documentation.

The right-hand side of Eq. 5.1 will often require computing spatial derivatives of fields. This is the dominant source of error in most simulations, as only spatially discrete data is available. For a grid with a lattice spacing \( \Delta x \), \textsc{CosmoGraph} contains functions to compute derivatives at up to \( \mathcal{O}(\Delta x^8) \).

As a last note about the solver implementation, the code does not presently take advantage of vectorization, with output from the GNU compiler tools demonstrating that no vectorization is performed. Rather, the code attempts to reduce the number of necessary calculations by computing all quantities dependent on field values at each point before proceeding to the next. Empirically, this results in somewhat slower
\[ y_a = y_p, y_f = 0 \]

\[ y_c = f(y_a) \]
\[ y_f \leftarrow y_c \]
\[ y_c = f(y_a) \]
\[ y_f \leftarrow y_c \]
\[ y_c = f(y_a) \]
\[ y_f \leftarrow y_c \]
\[ y_c = f(y_a) \]
\[ y_f \leftarrow y_c \]

\[ y_c = f(y_a) \]
\[ y_f \leftarrow y_c \]
\[ y_c = f(y_a) \]
\[ y_f \leftarrow y_c \]
\[ y_c = f(y_a) \]
\[ y_f \leftarrow y_c \]

Figure 5.3: The RK4 integration routine implemented in the **RK4Register** class. Different colors represent locations of arrays, or registers, in memory. Bold text indicates routines that need to be implemented by code making use of the **RK4Register** class. Further documentation of the integration routine is included in the codebase.

Performance (roughly \(\mathcal{O}(5 - 10\%)\)) than codes such as the McLachlan module in the Einstein Toolkit (ETK). However, as a number of additional parameters (such as ADM variables) are not computed during simulations, memory utilization is found to be roughly half that of the ETK.

In order to measure efficiency of the implementation, one common benchmark is strong scaling, which examines code ‘speedup’ as resources increase but problem size remains constant. This is shown in Figure 5.4 for a vacuum simulation of 5 iterations on a grid with a resolution of \(N^3 = 256^3\). The time taken to run on 16 cores relative to the time taken to run on more cores is plotted as a measure of code performance.
speedup. Significant code speedups are found for up to \( \sim 100 \) cores, however runs beyond this point either only benefit marginally or do not benefit.

![Strong scaling of CosmoGRAPH](image)

Figure 5.4: Strong scaling of CosmoGRAPH on a 512-core ESM node at the Bridges cluster at the Pittsburgh Supercomputing Center. The red line with dots as data points indicates measured performance, while the black solid line indicates theoretical optimal speedup.

### 5.1.2 Additional Implementation Details

A variety of additional features and design choices exist in CosmoGRAPH for performance, stability, and to explore the behavior of different numerical approaches. Several of these methods are detailed here, some of which are common among numerical relativity codes, and some of which are perhaps unique to CosmoGRAPH.

One of the more mundane of these aspects is the implementation of numerical dissipation, often attributed to Kreiss and Oliger [96]. The general idea is to add a dissipative term to each field being evolved using finite difference methods, at an order higher than that of the finite difference method itself. Such a technique has been demonstrably effective at reducing the appearance of high-frequency numerical
error, resulting in appreciably longer evolutions for certain systems [69]. For a method of order $O(\Delta x^p)$, the dissipative operator should be at least of order $p + 1$. For a method of order $p = 2(r - 1)$, the dissipation operator of order $2r$ is given by

$$Q = \sigma \frac{(-1)^r}{2^{2r}} \Delta x^{2r-1} D_+ D_-$$

(5.2)

for a dissipation strength parameter $\sigma > 0$, and upwind and downwind numerical stencils

$$D_+ f = \frac{(f(x + \Delta x) - f(x))/\Delta x}{\Delta x}$$

(5.3)

$$D_- f = \frac{(f(x) - f(x - \Delta x))/\Delta x}{\Delta x}.$$

(5.4)

As CosmoGRaPH was designed with a goal of comparing perturbative approximations, or solutions to the linearized Einstein equations, CosmoGRaPH also implements an option for evolving the linearized Einstein equations. This is relatively straightforward to accomplish in the reference formulation, involving the removal of all terms containing a multiplication of difference variables. The comparison is, however, not perfect; nonlinear metric inverses and other quantities accurate to second-order are still computed in some places. Thus the linearized evolution in CosmoGRaPH may contain differences from Newtonian or perturbative codes.

A final noteworthy feature of CosmoGRaPH is its implementation of a highly memory-efficient integrator. Although use of this incurs a significant speed penalty, the code contains an integrator requiring only a single $O(N^3)$ register of memory for
each field, regardless of method order. This integrator has been demonstrated to use roughly a factor of 4 less memory than the standard integration technique detailed in Fig. 5.3, and resultantly an order-of-magnitude less memory than the ETK code. Such an integration routine can in principle benefit codes running in memory-limited environments, such as on accelerators (GPUs).

This integrator was first implemented in a separate code for integrating the special relativistic Euler equations, also using an explicit finite-difference method, in [97]. The improvement made over standard RK4 integrator implementations is to take advantage of the local nature of finite differencing, and preserve only the local data necessary for performing the RK4 calculation. A ‘wedge’ of 2-dimensional slices is created to temporarily store intermediate data. The data is replaced as the code loops over the third dimension, with data in the grid being actively replaced with ‘final’ calculations once the grid data is no longer needed for computing. A more detailed visualization and textual writeup of the idea can be found in the code documentation. The method is implemented in a special (currently stale), wedge branch of the code.

5.2 Code Tests

A vital part of software development is ensuring the correct behavior of the code by performing a series of tests. This is important not only for verification of code written, but to ensure that future changes do not introduce regressions or bugs. COSMOGRAPH therefore includes several unit tests and test configuration files. A script was created to run some of these tests, which is automatically run by the continu-
ous integration platform TRAVIS-CI when changes are made to the code. However, even with tests that attempt to determine whether code changes affect output, additional work must be done to ensure the code output is both representative of a physical, continuum solution, and that solutions are indeed solutions to the Einstein field equations.

To this end, and of utmost importance for any numerical integration routine, is checking for convergence. Such checks are the primary means of verifying that solutions are approaching continuum solution as resolution is increased, especially when no analytic solution is available. Calculations performed without such checks are not usually meaningful, as any error due to finite resolution has not been quantified. Such checks are straightforward for grid-based codes, although have proven more difficult for N-body simulations, where the errors introduced due to the finite number of particles are not well-understood. Indeed, only quite recently has progress been made understanding under what conditions SPH N-body codes converge [88].

For the grid-based codes commonly found in numerical relativity, discretization approximations are made in both spatial and time domains, so convergence should be checked in each case. Given a method of order $\Delta x^p$ (and likewise with $\Delta t$), a numerical solution $\bar{y}$ should differ from the continuum solution $y$ by some amount proportional to this error, so that

$$y = \bar{y}(\Delta x) + \Delta x^p \epsilon_p + \Delta x^{p+1} \epsilon_{p+1} + \ldots,$$  \hfill (5.5)

where the $\epsilon_p$ are error functions at a given order and correspond to terms in a power
series expansion of the solution. Performing a calculation at three different resolutions, $\Delta x_1$, $\Delta x_2$, and $\Delta x_3$, the convergence factor can be defined in terms of these resolutions, and independent of the solutions $y$ and $\bar{y}$,

$$c = \frac{\bar{y}(\Delta x_1) - \bar{y}(\Delta x_2)}{\bar{y}(\Delta x_2) - \bar{y}(\Delta x_3)} \sim \frac{-y + \Delta x_1^p \epsilon_p + y - \Delta x_2^p \epsilon_p}{-y + \Delta x_1^p \epsilon_p + y - \Delta x_2^p \epsilon_p}$$

$$= \frac{\Delta x_1^p - \Delta x_2^p}{\Delta x_2^p - \Delta x_3^p}. \quad (5.6)$$

For CosmoGRAPH, good agreement can generally be found between the predicted and observed convergence rates, according to the integrator order being used.

In Figure 5.5 an explicit test of convergence is presented for a spacetime with only large-scale density fluctuations. A random realization of a spacetime with only $k = 1$ modes is chosen. The runs converge as expected: increasing the simulation resolution decreases the error according to the theoretical convergence rate for 8th order finite difference stencils. A comparison is also made to the standard BSSNOK (non-reference metric) formulation for small-amplitude fluctuations. For this system, the standard BSSNOK equations have reached the point where they cannot become more accurate due to truncation error, and thus fail to demonstrate meaningful convergence.

### 5.2.1 Apples with Apples Tests

While tests of numerical convergence can be used to check whether or not a solution is converging to a continuum solution, they will not necessarily determine whether or not the correct equations have been solved. Incorrect equations due to missing
Figure 5.5: Constraint violation amplitudes and the convergence rate $c$ for a universe with a dipole fluctuation. Constraint violation is presented for runs with a small-amplitude fluctuation, with $\sigma_\rho/\rho \times 10^{-5}$. Red lines (open shapes) are from runs utilizing the reference formulation, and green (arithmetic symbols) a non-reference formulation. The convergence rate of a run with a moderate-amplitude fluctuation ($\sigma_\rho/\rho \times 10^{-3}$) is also shown. Runs are performed at resolutions of $N^3 = 20^3$, $30^3$, and $40^3$ (light circles/slashes, medium squares/plus, and dark diamonds/x’s, respectively). A black dashed line indicating the theoretical convergence rate is also shown. For the small-amplitude fluctuations, the reference formulation can be seen to have smaller error and converge correctly, while precision error dominates the non-reference formulation, resulting in larger error and preventing correct convergence for.
terms, sign errors, or other such errors can nevertheless exhibit correct convergence behavior.

Thus, in addition to checking for numerical convergence, two further tests should be performed for a code: ensuring the physical and algebraic constraint equations remain small as simulations progress, and performing test simulations of spacetimes with known, analytic solutions. Performing these tests has been recognized as such an important practice that a standard set of tests has emerged: the ‘Apples with Apples’ (AwA) tests \[69\]. These tests are performed in different regimes, where the dynamics of the system is dominated by the behavior of different metric components or gauge variables. These include stability tests, gauge tests, and physical field configurations, some of which are known to be problematic for BSSNOK formulations.

The first two of these tests are of particular interest for CosmoGRaPH, not only because they can be run in synchronous gauge (which is used in this work for studying cosmological spacetimes), but also because of their ability to probe the reference metric formulation. These tests are designed such that the amplitudes of quadratic terms in the equations of motion will be at the level of truncation error around a flat, Minkowski spacetime. However, in the reference formulation, there is no ‘zeroth-order’ contribution from flat space, so the corrections from quadratic terms will be resolved. In this case, it is more important to verify that the constraint violation remains small, and that the simulation is stable, rather than checking for agreement with an approximate analytic solution.

All of the AwA tests are performed on a periodic spacetime. The dynamics are typically resolved in one or two dimensions by \( N = 50\rho \) points, with \( \rho \in \{1, 2, 4\} \), and
in the other two dimensions (or dimension) by a minimal number of points, \( N = 4 \).

Tests are also run for a large number of box-crossing times, and can be performed for rotations of the grid. The maximum absolute constraint violation (\( L_\infty \) norm) is generally presented in these tests, with the magnitude of vector constraints presented as \( M = \sqrt{\sum_i M_i M_i} \), and similarly for \( G \). Unless otherwise stated, results also make use of \( \mathcal{O}(\Delta x^8) \) accurate finite differencing stencils.

The first of these tests is coined the ‘robust stability’ test, and examines the behavior of small fluctuations (resembling high-frequency numerical error) around a flat spacetime. The metric in this case is given by the Minkowski metric plus these small fluctuations. A random number \( \epsilon \in (\pm 10^{-10}/\rho^2, 10^{-10}/\rho^2) \) is added to each variable. The metric is then evolved for \( 500\rho \) steps with \( \Delta t = \Delta x/10 \). The output from this test is checked to ensure that error growth is not superexponential, and that the rate of error growth does not increase as resolution increases. Results of this test for the CosmoGRAPH code are presented in Fig. 5.6.

Results from the robust stability test are presented for several resolutions and for several schemes attempting to minimize the constraint violation, including ‘K-damping’ (Eq. 2.45), A-adjusted terms (Eq. 2.54), and numerical dissipation (Eq. 5.2). For this test, the K-damping scheme does not improve stability as expected when the spacetime is not expanding, as \( K \) is not negative. The A-adjusted formulation does demonstrate a brief period of reduced constraint violation, however error growth is subsequently seen. The addition of explicit numerical dissipation then drastically improves the behavior of the system as would be expected. Finally, data from a non-reference formulation is included. The behavior of the non-reference formulation
Figure 5.6: Constraint violation and deviation from an analytic solution for various resolutions and damping schemes. Red lines (open circles, open squares, and open diamonds) correspond to resolutions $\rho = 1, 2, 4$; green lines (solid triangle) the A-adjusted formulation with $\rho = 4$ and $c_H = 1$; cyan (solid circles) K-damping with $\rho = 4$ and $\alpha_H = 1$, blue (solid squares) including numerical dissipation with $\rho = 4$ and $\sigma = 1$, and black (‘×’ symbols) a ‘standard’ (non-reference-metric) BSSNOK implementation. For reducing numerical noise of this type, numerical dissipation is seem to perform best. The reference formulation can also be seen to enforce algebraic constraints with significantly improved precision.
is very similar, however the algebraic constraints explicitly enforced in the code are seen to be substantially smaller for the reference formulation.

The next test is a plane wave of small amplitude, corresponding to an analytic solution of Einstein’s equations linearized around a flat metric, and thus an approximate solution to the full nonlinear equations. The amplitude of the wave is generally taken to be small enough that nonlinear corrections to the behavior will be at the level of roundoff error for a standard, non-reference 3 + 1 formulation. The solution at all times is given by the metric

\[
ds^2 = -dt^2 + dx^2 + (1 + H)dy^2 + (1 - H)dz^2,
\]

with

\[
H = A \sin(2\pi(x - t)).
\]

The value of \(A\) here is taken to be \(10^{-8}\), and the simulation run for 1000 box-crossing times and checked against the analytic solution. As this metric is not an exact solution to the Einstein equations, perfect agreement is not expected as resolution is increased, especially in a reference formulation where the nonlinear behavior should be resolved. After a long period of evolution, any initial constraint violation may grow or propagate if the system is not forced to a constraint surface. Such behavior is indeed seen in Fig. 5.7 with solutions converging away from the analytic solution and developing an overall offset and higher-frequency residual. Despite the apparent convergence to a solution other than the analytic solution, this deviation is not expected to be physical.
due to the inexact initial conditions used.

Next are two ‘gauge wave’ tests - solutions that can be mapped to Minkowski space via a coordinate transformation, but whose metric components nevertheless demonstrate a wavelike behavior. These metrics are of the form

\[ ds^2 = (1 - H)(-dt^2 + dx^2) + dy^2 + dz^2, \quad \text{and} \]
\[ ds^2 = -dt^2 + dx^2 + dy^2 + dz^2 + H(dt - dx)^2, \]

with \( H \) given by Eq. 5.9. These tests tend to pose a more significant challenge for BSSNOK codes due to the nontrivial geometry of the spacetime slices, which leads to instability [98]. In this case, both numerical dissipation (with \( \sigma = 1 \)) and higher-order stencils can be used to substantially lengthen the run time of the simulation. Nevertheless, only 15–30 box-crossing times elapse before the runs break down. Plots of the constraint violation amplitude and deviation from the analytic metric can be found in Figures 5.8 and 5.9.

### 5.2.2 Optical Component Integration and Testing

As a set of coupled ordinary differential equations, the optical scalar equations are relatively straightforward to integrate once the Weyl (or Riemann) tensor has been computed. In order to test the behavior of the integrator in COSMOGRAPH, the optical scalar equations are integrated through several analytic metrics that are relatively easy to comprehend. Because integration through a numerical spacetime is also necessary, metric quantities off of grid points will need to be computed, re-
Figure 5.7: Constraint violation and deviation from the approximate analytic solution for the linearized wave test. Red circles, green squares, and blue diamonds respectively correspond to $\rho = 1, 2, 4$. This test used 8th-order stencils, no dissipation or constraint damping, and the reference metric formulation. The solution can be seen to converge, although not precisely to the linearized analytic solution.
Figure 5.8: Constraint violation and deviation from an analytic solution for various resolutions for the gauge wave test. Colors and shapes are as in Fig. 5.6.

requiring an interpolation scheme. At the time of this writing, CosmoGRapH uses only simple linear interpolation, accurate to $O(\Delta x^2)$. The accumulated error in this scheme is therefore $O(\Delta x)$. In principle the interpolation and integration order can be improved, although in practice it has not yet been necessary because results have converged sufficiently quickly.

To help quantify the accuracy of the integrator, several analytic metrics are examined, including pure-FLRW (non-zero Ricci scalar), the Kasner metric (non-zero Weyl scalar), and a sinusoidal mode (non-zero spatial Christoffel symbols). The sinusoidal mode can also be used to quantify inaccuracy due to interpolation. For these metrics, convergence is established as expected, and their symmetries are exploited to check...
Figure 5.9: Constraint violation and deviation converging to an analytic solution for various resolutions for the shifted gauge wave test. Colors and shapes are as in Fig. 5.6 for any grid effects. These tests utilize time-reversed integration with timesteps of $\Delta t = 0.001, 0.0005, \text{ and } 0.00025$, in units where the FLRW scale factor is unity at $t = 1$.

5.2.2.1 Matter-dominated FLRW

Convergence and agreement with the matter-dominated FLRW solution obtained in Sec. 4.4 is demonstrated in Fig. 5.10. The convergence rate agrees with the theoretical behavior of a first-order scheme, for which $c = 2$. In order to ensure correctness of the integrator, this test is also performed for photons traveling in several directions, including off-axis. As expected due to imperfect cancellation of terms, the off-axis
calculations exhibit larger errors while still converging to the correct solution. Errors are also found to be of order $\Delta t$, as expected from the integration method order.

![Graphs showing photon energy, beam width, and energy difference over simulation time.](image)

Figure 5.10: Results from raytracing through a matter-dominated, homogeneous FLRW spacetime, which demonstrate convergence and agreement with analytic results. Lines from runs with timesteps $\Delta t = 0.001$ (red, dotted), 0.0005 (green, dashed), and 0.00025 (solid, blue) are shown in the top plots, for both beam width $\ell$ and energy $E$. Convergence of these quantities is seen in the bottom plots, indicating $c = 2$ as expected. Orange, dashed lines are the difference between the larger timesteps, and solid cyan the difference between the smaller timesteps, multiplied by the convergence factor.

### 5.2.2.2 Anisotropic Expansion and the Kasner Metric

Integration through the Kasner metric provides a test of the behavior of the screen vectors and Weyl calculation. The Kasner metric is a vacuum solution to Einstein’s equations sometimes found in cosmological calculations, particularly near singular solutions. Contrasting the matter-dominated FLRW solution, the lack of matter
(and singularities) in a Kasner spacetime means that the Ricci optical scalar will be zero, and thus will not contribute to the dynamics of the beam morphology. However, for this metric the Weyl optical scalar is non-zero, so the system exhibits non-trivial behavior.

The Kasner metric is given by

$$g_{\mu\nu} = \text{diag} \left(-1, a_x^2(t), a_y^2(t), a_z^2(t)\right),$$  \hspace{1cm} (5.12)

and the extrinsic curvature is given by

$$K_{ij} = -a_i \dot{a}_i \delta_{ij} \hspace{1cm} (5.13)$$

$$K^i_j = \gamma_{ik} K^k_j = \frac{\dot{a}_i}{a_i} \delta_j^i, \hspace{1cm} (5.14)$$

making a special note that no summation is implied here. The lack of summation will also be the case in the derivation that immediately follows. For this metric, the non-zero Christoffel symbols are

$$^{(4)}\Gamma^{0}_{ij} = a_i \dot{a}_i \delta_{ij} \hspace{1cm} (5.15)$$

$$^{(4)}\Gamma^{i}_{j0} = ^{(4)}\Gamma^{i}_{0j} = \frac{\dot{a}_i}{a_i} \delta_j^i, \hspace{1cm} (5.16)$$

with all spatial, 3-Christoffel symbols being zero. Lastly, the nonzero components of
the Riemann tensor are

\[ R_{i00j} = a_i \ddot{a}_i \delta_{ij} \]  
(5.17)

\[ R_{ilmj} = -a_m \dot{a}_m a_i \dot{a}_i \delta_{lm} \delta_{ij}, \]  
(5.18)

from which the Weyl optical scalar terms are found to be non-zero,

\[ \frac{1}{2} W^\Sigma_{AB} = -a_x \ddot{a}_x \varsigma_{[01]}^A \varsigma_{[01]}^B - a_y \ddot{a}_y \varsigma_{[02]}^A \varsigma_{[02]}^B - a_z \ddot{a}_z \varsigma_{[03]}^A \varsigma_{[03]}^B \]

\[ + a_x \dot{a}_x a_y \dot{a}_y \varsigma_{[12]}^A \varsigma_{[12]}^B + a_x \dot{a}_x a_z \dot{a}_z \varsigma_{[13]}^A \varsigma_{[13]}^B \]

\[ + a_y \dot{a}_y a_z \dot{a}_z \varsigma_{[23]}^A \varsigma_{[23]}^B. \]  
(5.19)

Given the Christoffel symbols computed above, the geodesic equations are

\[ \frac{dV^i}{dt} = \left( \frac{2 \dot{a}_i}{a_i} + \sum_j a_j \dot{a}_j (V^j)^2 \right) V^i \]  
(5.20)

\[ \frac{dE}{dt} = -E \sum_j a_j \dot{a}_j (V^j)^2. \]  
(5.21)

A particularly useful feature of the geodesic equations in this spacetime can be seen by noting that the direction of photon velocities should not change, although the magnitude should. This provides an additional check as the simulation progresses. As noted, this is a vacuum solution with zero stress-energy, so \( T_{\mu\nu} = 0 \), indicating that \( \mathcal{R} = 0 \).

For this test, the particular Kasner solution chosen is \( a_i = t^{p_i} \), with \( p_x = 2/3 \), \( p_y = 2/3 \), and \( p_z = -1/3 \). Integration is performed with a velocity component in the
z direction and $x$-$y$ plane, and results are plotted in Figure 5.11. The test is performed with the velocity in the $x$-$y$-plane rotated by various angles. Computed quantities should be identical due to the symmetry of the system, and can therefore checked for agreement. Pairs of screen vectors with differing orientations are also integrated to ensure the result does not depend on the particular screen vectors chosen.

Figure 5.11: As with the FLRW case presented in Fig. 5.10, the top panels show agreement between runs of $E$ and $\ell$ for the Kasner metric universe for three different timesteps, while the bottom panel demonstrates convergence.

### 5.2.2.3 Sinusoidal Mode

In order to test convergence properties of the geodesic integrator in a discretized spacetime, and therefore properties of the interpolation scheme, integration through a spatially inhomogeneous metric is necessary. One such example is a metric with a
perturbation in some direction,

\[ ds^2 = -dt^2 + (1 + \epsilon(x)) \, dx^2 + dy^2 + dz^2 , \quad (5.22) \]

so that \( \gamma_{ij} = \delta_{ij} + \epsilon(x) \delta_i^x \delta_j^x \), and \( \gamma^{ij} = \delta^{ij} - \frac{\epsilon(x)}{1+\epsilon(x)} \delta_i^x \delta_j^x \). Although this metric may correspond to a solution for some (perhaps unphysical) matter source, the particular matter source does not need to be specified to integrate the geodesic equations.

Choosing a metric with fluctuations of a fixed scale is also a useful proxy for exploring behavior in a more realistic cosmological spacetime, since the scale of the test metric fluctuations can be chosen to be similar to the scale of fluctuations in a cosmological spacetime. Running this test at different resolutions may also provide some insight into which regimes accurate integration can be performed. Convergence properties can also be studied using this metric rather than using more computationally expensive, fully dynamical cosmological simulations.

The only nonzero 3-Christoffel symbol for this spatial metric is given by

\[ \Gamma^x_{xx} = \frac{1}{2} \frac{1}{1 + \epsilon} \partial_x \epsilon . \quad (5.23) \]

Choosing \( \epsilon(x) \) in order to study the behavior of the integrator due to fluctuations of particular wavelengths, a sinusoidal function can be chosen,

\[ \epsilon(x) = \epsilon_0 \sin(2\pi x / L) , \quad (5.24) \]
so that

\[ \Gamma_{xx}^x = \frac{\pi \epsilon_0 \cos(2\pi x/L)}{L \left(1 + \epsilon_0 \sin(2\pi x/L)\right)} \]  

(5.25)

and correspondingly,

\[ \Gamma_{xxx} = \frac{1}{2} \partial_x \epsilon(x) = \frac{\pi}{L} \epsilon_0 \cos(2\pi x/L). \]  

(5.26)

The convergence behavior of the integrator is compared both using this analytic expression, and a ‘lattice’ spacetime with metric values interpolated from nearby points. Given a lattice spacing \( \Delta x \) and ray position \( X \), the interpolated values will need to be calculated from \( \Delta x \lfloor X/\Delta x \rfloor \) and \( \Delta x \lceil X/\Delta x \rceil \). For this metric, \( K = 0 \), so the photon energy should not change. The only velocity component with a non-zero source term is the velocity in the \( x \)-direction,

\[ \frac{dV^x}{dt} = (3) \Gamma_{xx}^x (V^x)^2. \]  

(5.27)

The Riemann tensor for this metric has no non-zero components, so the Weyl and Ricci optical scalars do not contribute to the beam morphology. However, the behavior of the photon trajectory itself can still be examined. As with the Kasner and FLRW tests, both the timestep \( \Delta t \) and resolution \( \Delta x = 10\Delta t \) are increased. Results from integrating this spacetime can be found in Figure 5.12.

At least one exact solution to the Einstein field equations exists in which an optical integration has been performed, the Meures-Bruni metric [99]. Verifying solutions converge to the analytic results for this metric, and for any other such metrics is a
Figure 5.12: As with the other raytracing tests presented in Fig. 5.10 and Fig. 5.11, the top panel above shows agreement between runs for $E$ and $\ell$ using the sinusoidal metric with three different timesteps, and the bottom panel demonstrates their convergence.

high priority for any work.
Chapter 6

An Overview of Applications

This chapter addresses the ability of the previously discussed relativistic techniques and code to obtain results accurate enough to compare to measurements in a cosmological setting. In order to both motivate the need for relativistic simulations and determine the accuracy required in order to resolve corrections to approximate schemes, this chapter begins with a discussion of the physics that is often neglected by approximate treatments. Subsequently, an overview of preliminary dust simulations performed using CosmoGRAPH is presented in order to not only demonstrate regimes where simulations are valid, but determine where the approach breaks down, and describe potential remedies.

Future observations are expected to place percent-level constraints on cosmological parameters \[100\] and perform sub-percent-level measurements of properties of systems, such as photometric redshifts \[101\]. It will be important to understand if, and how, corrections to approximate calculations can affect the interpretation of such measurements. Even if such corrections are large, they could be stochastic in nature,
and ‘average away’ – in which case statistical statements from approximate methods could prove fairly robust. However, it is also possible that relativistic corrections are biased in a coherent way, leading to a systematic misinference of inferred cosmological parameters.

It is useful to perform a preliminary calculation to explore the scales on which a perturbative or Newtonian approach might break down, or in which regimes corrections might be largest. A straightforward way to obtain an order-of-magnitude estimate of the amplitude of corrections is to examine the extent to which the metric potential is expected to deviate from a Newtonian approximation. In the Newtonian picture of a ΛCDM universe, the Newtonian potential, $\Phi_N$, is given at zeroth-order by Newton’s equation,

$$\nabla^2 \Phi_N = 4\pi a_{\text{FLRW}}^2 \delta \rho,$$

(6.1)

where $a_{\text{FLRW}} = 1$ today, and $\delta \rho = \rho - \bar{\rho}$, with $\bar{\rho}$ the volume-averaged density. In Fourier space, the amplitude of the gravitational potential is therefore determined by the relative size of $\delta \rho$ and the inverse length scale $k^2$. For density fluctuations with an RMS amplitude of $\sigma_\rho = 0.1$ at scales of order $k^{-1} \sim 100h^{-1}$ Mpc [15], the amplitude of deviations of the metric is found to be a few parts in $10^4$. The amplitude remains at this level up to scales of a few gigaparsecs, and shrinks at smaller scales.

Corrective terms of this amplitude may arise in the form of derivatives of the metric or multiplications of terms by the metric, for example terms of the form $\Phi_N \nabla^2 \Phi_N$ or $\nabla_i \Phi_N \nabla^i \Phi_N$. A perturbative approach has previously attempted to take such effects into account, linearizing after considering metric quantities to be of order $\epsilon$, and
differentials to be of order $\epsilon^{-1/2}$ [102]. However, a comparison between Newtonian calculations, linearized calculations (in any form), and fully relativistic work has yet to be performed.

Rough arguments can be given in favor of an increased or decreased amplitude of nonlinear corrections, however modeling will be required to precisely determine the impact of these effects on the metric quantities. Additional effects neglected in a perturbative treatment can be found in the literature. These include, for example, so-called ‘frame-dragging’ effects that arise at linear order in a perturbative expansion [103], and nonlinear corrections due to the presence of relativistic sources such as neutrinos [104]. These corrections are sourced by anisotropic stress and momentum, and are therefore expected to be of order the amplitude of peculiar velocities, which are observed to be $v/c \sim 10^{-3}$.

Work on fully nonlinear relativistic dynamics has been able to approach cosmology from the opposite, completely non-perturbative direction. Numerical studies of black hole lattices have been performed on cosmological scales, effectively comprising truly relativistic cosmological ‘N-body’ simulation [51]. In these simulations, the matter content of the universe was placed in $O(5 - 10)$ black holes, regularly or irregularly positioned in the spacetime. These models found a disagreement between simulated metric components and a corresponding FLRW model to be of order 25%.

No matter the approach used to study the spacetime metric, any corrections to an approximate treatment of the metric can result in corrections to predictions for observable quantities. However, additional corrections may enter due to approximations made when evaluating the optical scalar equations in a perturbative setting, and
approximations inherent in the optical scalar equations themselves. Further approximations may be made when performing statistical operations, such as commuting averaging and differencing, or averaging in a gauge-dependent manner, resulting in further inaccuracies. A number of such effects have been examined in the literature for specific measurements or calculations. These include, for example, $\gtrsim 10\%$ corrections to bispectra and cross spectra [105,106], percent-level corrections to inferred cosmological parameters [107], increased variance in measurements [108], and more.

While corrections have been studied numerically and analytically in a fully non-linear setting, there are also observed features of the Universe indicating the potential for relativistic effects to be significant. Black holes have been observed with masses of order $10^{10}M_\odot$, requiring the accretion of all matter contained in 1Mpc$^3$ volumes [109]. The dynamics leading to the formation of such objects, and the resulting influence of these objects on the evolution of the Universe remains poorly understood and is not well-modeled in a Newtonian picture. In addition to such objects, significant local inhomogeneities have been observed on large scales, such as coherent ‘great wall’-type structures at scales of 2-3 Gpc [110].

The potential for relativistic physics to affect both measurements and their interpretations should be clear from these examples – however, the magnitude of such corrections is less clear. Given the above estimates, the accuracy required for any method attempting to address these problems should be at least part-in-$10^4$-level in order to make predictions that can be reliably compared to approximate calculations. The remaining sections of this chapter are devoted to describing some applications of the techniques presented here and their ability to achieve this level of accuracy.
6.1 Variants of a Fiducial Model

Cosmological simulations using the method of Chapters 2 and 3 can be run for a standard — fiducial — set of parameters. The error and convergence can be explored in detail as the number and amplitude of modes in a volume are varied. Several statistical quantities will be referenced when comparing results. These include conformal (volume-weighted) averages,

\[ \bar{f} \equiv \frac{\int dx \sqrt{\gamma} f}{\int dx \sqrt{\gamma}} \approx \sum_{x_i} e^{6\phi_i} f_i, \quad (6.2) \]

and volume-weighted standard deviations,

\[ \sigma_f \equiv \sqrt{\frac{N}{N - 1} \sum_{x_i} e^{6\phi(x_i)} (f(x_i) - \bar{f})^2} \sum_{x_i} e^{6\phi(x_i)}, \quad (6.3) \]

of fields \( f \) on spatial slices. Constraint violation amplitudes may also be presented relative to the ‘scale’ of the violation amplitudes. The scale is determined by the rooted sum of squares of individual terms in the constraint equations, and notated using brackets, ie.

\[ [\mathcal{H}] = \sqrt{(\bar{D}^2 e^\phi)^2 + \left( \frac{e^\phi}{8} \bar{R} \right)^2 + \left( \frac{e^{5\phi}}{8} \bar{A}_{ij} \bar{A}^{ij} \right)^2 + \left( \frac{e^{5\phi}}{12} K^2 \right)^2 + \left( 2\pi e^{5\phi} \rho \right)^2} \quad (6.4) \]

for the Hamiltonian constraint. When presented relative to this scale, the amplitude very roughly corresponds to the fractional deviation from a constraint surface.

The fiducial parameters used here correspond to a spacetime with a volume \( V^{1/3} = \)
$L^3 = (H^{-1}/2)^3$, resolution of $N^3 = 128^3$, timestep $\Delta t = \Delta x/10$, and 6th or 8th-order finite difference stencils. Initial conditions are set according to the prescription in Section 3.2. The power spectrum amplitude (Eq. 3.20) chosen corresponds to an RMS density of $\sigma_\rho/\bar{\rho} = 0.04$, with a peak frequency of $k = 7/128\Delta k$, and modes initialized up to $k = 10/128\Delta k$. The shortest wavelengths in this model will therefore be resolved with around 12 points.

In order to see how the error scales as modes are resolved by different numbers of points, the spectrum cutoff can be varied. Both the error growth and statistical behavior of the metric and density fluctuations are shown in Figures 6.1 and 6.2. As a proxy for simulation time, these values are plotted as a function of the average conformal factor on the spatial foliation, or roughly half the number of e-folds of expansion ($a_{\text{FLRW}} = e^{2\phi}$). It is important to note that the statistics presented here are gauge-dependent, and thus do not necessarily reflect physical properties of the spacetime.

The increase in error due to poorly-resolved modes is the dominant contribution to the error in these diagrams. In synchronous gauge, where fluctuations in metric quantities can grow quite large, this can be especially problematic. Working in an alternative gauge, such as Harmonic gauge or ‘1+log’ slicing gauge, will tend to prevent the growth of large-amplitude fluctuations, and thus growth of errors. Results from this analysis nevertheless suggest that modes will need to be resolved by $O(10)$ points in order to maintain the desired accuracy. While this may improve in another gauge, the problem may also worsen when simulations are run for a longer time.

As previously noted, coordinate singularities can form as a result of the fluid
Figure 6.1: The properties of the spacetime, and constraint violation for various spectrum cutoffs, are shown up to an e-fold of expansion. The cutoffs are, from bottom to top in all plots, $k_{\text{cut}}/\Delta k = 2, 4, 8, 10, 12, 14, 16, 20, 40$, colored from blue to red respectively. On the constraint violation plots, dashed lines indicate the maximum error found in the spacetime, solid lines the mean, and shaded lines one standard deviation around the mean. Statistical quantities shown are the normalized RMS density fluctuation, RMS expansion rate, and RMS 3-Ricci scalar. The error remains at a part-in-$10^4$-level for cutoffs below $k/\Delta k \sim 20$ for the duration of the simulation, but may continue to increase beyond this point.
Figure 6.2: Statistical properties and constraint violation of a cosmological spacetime are shown for the fiducial model with the spectrum amplitude varied, for up to an e-fold of expansion, as in Figure 6.1. Each color indicates a run with a different spectrum amplitude, whose amplitudes correspond to a $\sigma_\rho/\bar{\rho}$ as shown in the top middle figure.
approximation and use of synchronous gauge. This problem should manifest on scales where multistreaming takes place, which are of order 10 Mpc, and should become increasingly worse at smaller scales. Such scales are not yet resolved in this model, due to both the spectrum cutoff and finite resolution used. As the resolution of simulations increases and this issue becomes significant, use of a non-singular gauge such as Harmonic gauge will likely be necessary, as well as a technique capable of resolving more of phase space, such as a Vlasov or N-body approach.

6.2 Comparisons to Linear Theory in Synchronous Gauge

A comparison to linear perturbation theory in synchronous gauge is also straightforward to obtain. The BSSN equations linearized around an FLRW solution are given by

\[
\partial_t \delta \rho = \bar{\rho} \delta K + \bar{K} \delta \rho
\]

\[
\partial_t \delta K = \frac{2}{3} \bar{K} \delta K + 4\pi \delta \rho
\]

for linear perturbations \(\delta K\) and \(\delta \rho\) around background FLRW quantities \(\bar{\rho}\) and \(\bar{K}\). These variables can be equated to variables in standard cosmological perturbation theory in synchronous gauge, such as [111], where the authors use \(\dot{h}\) as the extrinsic curvature, \(\delta K = -\dot{h}/2\), and \(\delta\) for the density contrast, \(\delta = \delta \rho/\rho\).
These are simple ODEs that can be integrated analytically, with solutions

\[
\begin{align*}
\bar{\rho} &= \frac{1}{6\pi t^2} \\
\bar{K} &= -\frac{2}{t} \\
\delta\rho &= \frac{2\delta\rho_0}{135t^3} (13122t^5)^{1/3} + 8) \\
\delta K &= \frac{8\pi\delta\rho_0}{45t^2} (486t^5)^{1/3} - 4),
\end{align*}
\]

in units where the initial Hubble scale is unity. So long as any contribution from \(\bar{A}_{ij}\bar{A}^{ij}\) is negligible, the full evolution equations for \(\rho\) and \(K\) remain a set of ODEs that can be integrated numerically.

Good agreement between simulated average values and FLRW (or background) predictions can be seen in Figure 6.3, although a small deviation can be seen that persists with changes in resolution. As this is a foliation-dependent average, this correction is not necessarily physically meaningful. The background quantities themselves are found to have been computed with an accuracy nearly at the level of working precision, as shown in Figure 6.4.

The dashed lines in the right panel of Fig. 6.5 depict approximate solutions for the fiducial model. The curves show that the metric values are centered about the linear-order predicted value. They agree even more closely when only the \(\bar{A}_{ij}\bar{A}^{ij}\) term is neglected, but still exhibit noticeable deviations. Due to the neglected \(\bar{A}_{ij}\bar{A}^{ij}\) term being positive-definite, simulated data should lie only below the approximate, ‘u’-shaped curve. A small violation of this relationship can be seen in the binned data, with several data points lying above the curve, indicative of a small amount of error.
Figure 6.3: Averaged quantities compared to a reference FLRW background model. Constraint violation is seen to converge to zero as expected. A small deviation from FLRW quantities is found that persists as resolution increases.

As the amplitude of metric fluctuations in synchronous gauge grow large, nonlinear corrections are also expected to increase. However, the amplitude of corrections (and numerical error) may be smaller in different gauges \[112\].
Figure 6.4: Agreement of reference FLRW values with analytic calculations.

Figure 6.5: The relationship between fluctuations in matter density and extrinsic curvature is shown at a time where $\bar{\phi} = 0.5$ (after one e-folding of evolution). The differences of metric values from a linear approximation are plotted for a given local density. The black dashed line (at zero) represents the linear-order analytic solution, and dashed purple the solution excluding only contributions from the $A_{ij} \bar{A}^{ij}$ term. Data from a simulation is also binned in a 2-D histogram. This data originates from a simulation with an intermediate value of inhomogeneity, $\sigma_\rho / \bar{\rho} = 0.038$. Local violations of the linear-order approximation are seen to be of $\mathcal{O}(5\%)$. 

100


6.3 Optical Integration

Before discussing the accuracy of the optical integrator in the cosmological model presented in the previous section, it is important to attach some intuition to observed quantities so that they can be qualitatively understood. Hubble diagrams can be constructed for observers in this spacetime, with angular-diameter distances converted to apparent magnitudes, \( m - M = 5 \log_{10} \left( D_A (1 + z)^2 / 10 \text{pc} \right) \). Observers are chosen to have velocities coincident with the fluid velocity, or zero velocity in synchronous gauge.

At ‘zeroth’ order, Hubble diagrams should appear very close to predictions from an FLRW model. In Figure 6.6, results from a simulation are presented, indicating agreement with this notion. The reference FLRW model is then subtracted off in Figure 6.7 in order to more clearly depict deviations from this model. Notably, there are several reference spacetimes that can be subtracted off, corresponding to the average density, expansion rate, or scale factor at any time throughout the simulation. These may all differ by some amount. Here, a model is chosen that agrees with the expansion rate on the initial slice.

For an observer whose local density is close to the average density on a spatial slice, intuition might suggest that local structure will not contribute appreciably to deviations of the average from an FLRW model. This expectation arises from the idea that, while photons probing over-densities in one direction may experience some effect, this will largely be canceled by photons probing under-densities in different directions. Nevertheless, to the extent that more over- or under-densities are present
Figure 6.6: A Hubble diagram according to an ‘average’ observer. The black dotted line indicates the prediction from a pure-FLRW model, many green dashed lines are derived from angular diameter distances computed along individual lines of sight, and the red line is the average along all individual lines of sight. The different lines are nearly indistinguishable, indicating good agreement.

near such an observer, there may be local fluctuations.

Two separate effects will contribute to the deviation of angular diameter distances from an FLRW model. The first of these effects comes from deviations of photon energy from FLRW predictions, which are sourced by fluctuations in the expansion rate, as described by Equation 4.18. While traversing regions with larger expansion rates, photons may be expected to undergo additional redshifting. The second effect can be seen to arise from the optical scalar equations. As photons probe denser regions, they undergo additional focusing, because the Ricci optical scalar increases with density. This causes beams of a larger area to be directed towards an observer,
and thus the angles subtended by objects to appear larger, resulting in a reduced angular diameter distance measurement.

In synchronous gauge, overdensities correspond to regions of increased $K$ (ie. $K$ closer to zero; thus regions with a decreased expansion rate), and underdensities to regions of decreased $K$ (or an increased expansion rate). An increase in density therefore corresponds to smaller angular diameter distance measurements, shifting the Hubble diagram residual down. However, it also corresponds to photons experiencing a smaller redshift, which tends to drive the diagram up. The effect from the reduction in redshifting dominates the behavior, creating a net increase in the measured angular diameter distance as a function of redshift, while underdensities have the opposite effect. In other gauges, such effects can be attributed to other dynamics. For example, in Poisson gauge (where effects are gauge-invariant to first order, and therefore can be interpreted as physical at this order), the dominant effect is attributed to peculiar velocities. In this case, observers in an overdensity see others collapsing towards themselves, resulting in a relative blueshifting of photons, while other effects are considered much smaller.

Agreement can be found between such intuition and numerical results. For an average observer, beams traversing individual geodesics trace out a distribution of angular diameter distances, the mean of which closely tracks the FLRW expectation at all redshifts. For overdensities and underdensities, an initial peak or dip can be seen, respectively, in Figure 6.7.

To conclude this section, two of the approximations made in the Dyer-Roeder scheme are tested. The Dyer-Roeder approximation is a phenomenological approxi-
Figure 6.7: Residual Hubble diagrams produced by integrating the optical scalar equations through an inhomogeneous universe. The initial RMS density fluctuation amplitude is $\sigma_\rho/\rho = 0.1$, which is somewhat larger than the fiducial model presented previously. By the end of the simulation, the amplitude has grown to $\sigma_\rho/\rho = 0.2$. The left figure is a Hubble diagram for an observer located at a position of ‘average’ density, and the right figure for an observer in an overdensity. Thin black lines depict angular diameter distances along several particular lines of sight for this observer. The black dashed line indicates the prediction from a pure-FLRW model. The solid red line indicates the average angular diameter distance of these rays, for which agreement with an FLRW model is seen. The statistical error – standard error in the mean – is shown at the one and two ‘sigma’ level by semi-transparent red shading, so the width of the red curve is indicative of the error. White dashed lines indicate the standard deviation of the distribution of magnitudes. Finally, the background shows a histogram of the magnitudes along all integrated lines of sight as a function of redshift.

Information describing relativistic effects on observables, which relies on several physical assumptions rather than a perturbative analysis [113]. The assumptions made are: (1) photons redshift according to an FLRW model, (2) the Weyl optical scalar does not contribute significantly to dynamics, and (3) that the Ricci optical scalar is given by the FLRW value reduced by a constant multiplicative factor.

Although the original Dyer-Roeder approximation holds that the Ricci optical scalar is given by the FLRW value reduced by a constant multiplicative factor, this as-
assumption has been relaxed in practice to allow the constant to vary both spatially and with redshift \[114\]. This constitutes more of a phenomenological re-parametrization, and is therefore not explored below. The remaining approximations are found to be accurate to a high degree of precision in this spacetime, however resolvable corrections can still be found.

The first assumption is that photons redshift according to an FLRW model. A straightforward way to test this is to examine photon redshift compared to the expansion rate, or density. In general, these values will be gauge-dependent, so in order to perform a conservative comparison, local values of the density are used. The deviation in this relationship is presented in Figure 6.8 and is seen to be of order part-in-\(10^3\) for individual curves. Nevertheless, the approximation is found to be substantially more accurate on average.

The second of these assumptions asserts that the contribution from Weyl shearing is negligible. In order to determine the contribution of the shearing, the magnitude of the contribution of the shearing relative to Ricci focusing, \(\sigma^2/R\), can be examined. The amplitude of this quantity is also plotted in Figure 6.8 from which it is seen to contribute near the part-in-\(10^5\) level.
Figure 6.8: Violations of Dyer-Roeder assumptions for the fiducial model, with an initial RMS density amplitude of $\sigma_\rho/\bar{\rho} = 0.1$. The left plot shows the fractional change in photon energy relative to an FLRW model. The right plot shows the relative contribution of shearing and Ricci focusing, $\sigma^2/\mathcal{R}$. The thick solid lines indicate median values, and the shaded band the extent of the interquartile ranges.
Chapter 7

Future Directions

Cosmological modeling in a fully relativistic setting will enable a more accurate and robust interpretation of cosmological observables. Such a tool can provide not only a standard for benchmarking the validity and accuracy of approximate schemes, but also new insight into the dynamics of relativistic systems in cosmology. Determining the importance of these effects will be necessary to probe physics of the dark sector, where accurate modeling will be required in order to differentiate between various models describing cosmological phenomena.

This thesis describes the formalism behind a fully relativistic framework for performing calculations in a cosmological setting and details of a code implemented within this framework. The accuracy and convergence properties of the code are examined and found to be capable of modeling cosmology with a level of accuracy necessary to probe physics beyond a Newtonian or perturbative setting.

Nevertheless, while the simulations presented in Chapter 6 are intended to mimic physics in a cosmological setting, they are not yet realistic enough to make obser-
vational predictions. The possibility of obtaining solutions with sufficient accuracy has been demonstrated, yet this is from the standpoint of numerical accuracy. As the importance of nonlinear gravitational interactions increases in a physical system, accurate calculations may also require resolving smaller scales in order to obtain realistic predictions for both physical and statistical effects at a desired level of accuracy. Work from Newtonian N-body simulations conservatively suggests that modeling scales from Gigaparsecs to sub-Megaparsecs with sub-percent accuracy will require trillions of particles [115], a resolution that has been attained only very recently [12–14].

Thus, as cosmology moves into an era with measurements of sub-percent-level accuracy, significant technical challenges still need to be overcome to perform cosmological modeling with sufficient resolution. Yet the necessary tools for the job have been developed, providing a critical link between observational measurements and their physical interpretation, and paving the way for future work in this field.
Bibliography


[61] E. Bentivegna and M. Bruni, “Effects of nonlinear inhomogeneity on the
no. 25, 251302, arXiv:1511.05124 [gr-qc].

from Homogeneity in an Inhomogeneous Universe,” arXiv:1608.04403
[astro-ph.CO].

[63] M. Alcubierre, A. de la Macorra, A. Diez-Tejedor, and J. M. Torres,
no. 6, 063508, arXiv:1501.06918 [gr-qc].

arXiv:1509.08354 [gr-qc].


[66] O. Sarbach and M. Tiglio, “Continuum and Discrete Initial-Boundary-Value
arXiv:1203.6443 [gr-qc].

Equations on the Computer*. Cambridge University Press, Cambridge, UK,
2010.

[68] M. Alcubierre, *Introduction to 3+1 numerical relativity*. International series of
https://cds.cern.ch/record/1138167

[69] M. C. Babiuc et al., “Implementation of standard testbeds for numerical
[gr-qc].

[70] J. D. Brown, “Covariant formulations of BSSN and the standard gauge,”

[71] T. W. Baumgarte, P. J. Montero, and E. Müller, “Numerical Relativity in
no. 6, 064035, arXiv:1501.05259 [gr-qc].

[72] E. Gourgoulhon, “3+1 formalism and bases of numerical relativity,”
arXiv:gr-qc/0703035 [GR-QC].


