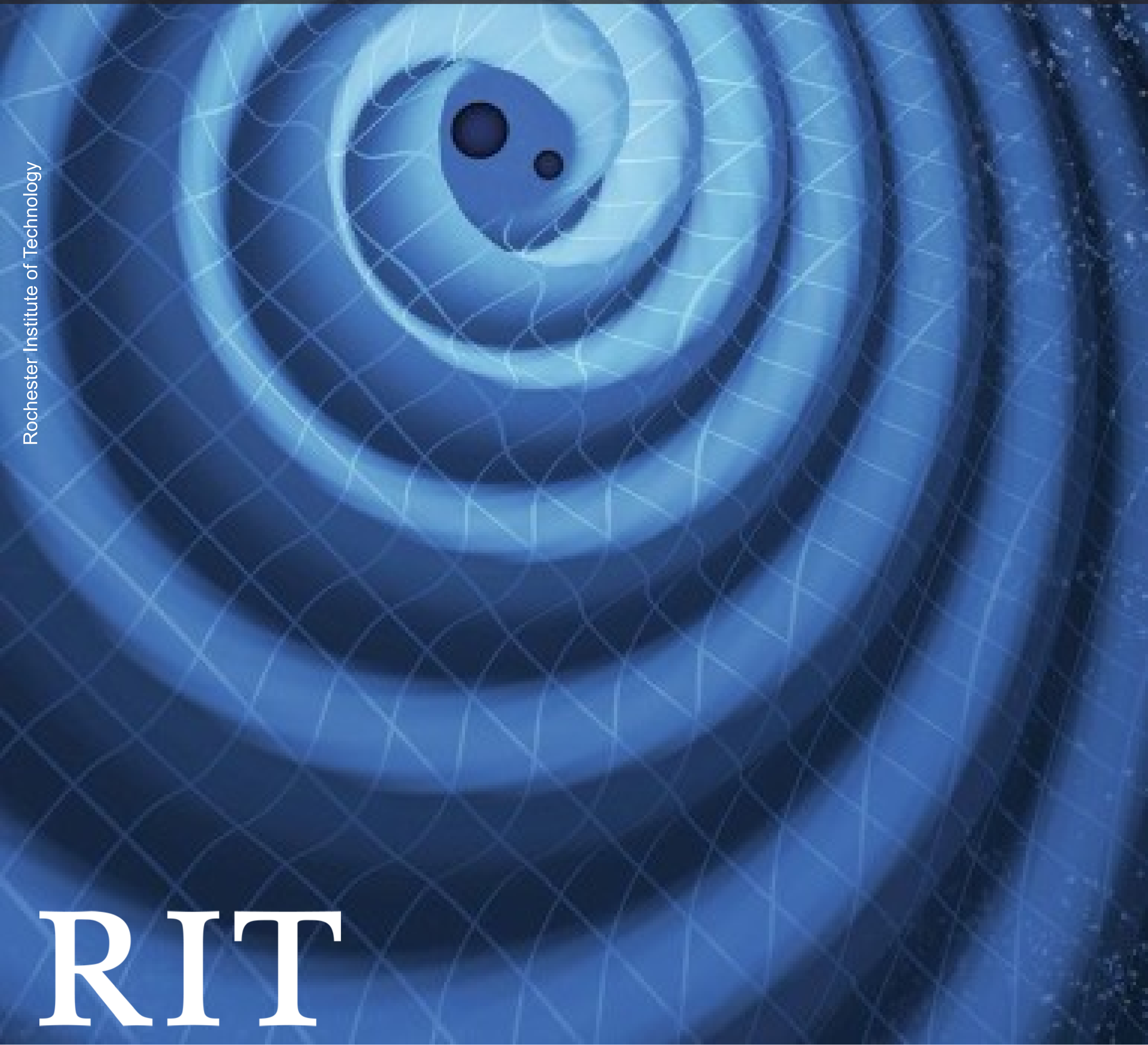
The Initial Data Problem of Numerical Relativity

Construction of Black-Hole Initial Data

Mathematical Modeling II

Mario L. Gutierrez Abed



Rochester Institute of Technology

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by

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Preface

In this report we investigate the initial data problem of numerical general relativity. After a brief introduction of some of the basic, most widely used ideas and formalisms of the field, we dive right into the issue of constructing initial data for black holes. We shall use the conformal transverse-traceless decomposition to tackle the Hamiltonian and momemtum constraints on a conformally-flat spatial geometry. Upon construction of Bowen-York puncture data for a single black hole, we observe the possible limitations of such model on the parameter space. In particular, we see that as the spin of the black hole is increased, the data loses regularity. Theoretically, such a shortcoming was to be expected, since it is known that a rotating Kerr black hole does not admit a conformally-flat spatial slice. This letter presents a "hands-on" calculation that exhibits the aforementioned drawback of the Bowen-York approach. The project will serve as a foundation for future work on initial black hole data on a conformally-Kerr spatial metric.

Mario L. Gutierrez Abed
Rochester, May 2021

Contents

Conventions

Metric signature	"Mostly plus" $(-+\cdots+)$
Einstein summation	"Downstairs" and "upstairs" indices are summed over; e.g., $X^i e_i = \sum_i X^i e_i$
Index convention	Standard convention whereby the letters $a-h$ and $o-z$ are used for 4-dimensional spacetime indices that run from 0 to 3, whereas the letters $i-n$ are reserved for 3-dimensional spatial indices that run from 1 to 3. Lowercase Greek letters are reserved for components in a chosen basis (see [26] for reference).
Dimensionless units	$G = c = 1$ (unless otherwise stated)
Cosmological constant	$\Lambda = 0$
Riemann curvature	$R(X,Y)Z = \nabla_X \nabla_Y Z - \nabla_Y \nabla_X Z - \nabla_{[X,Y]} Z$
(In components)	$R^d{}_{abc} = \partial_b \Gamma^d_{ac} - \partial_c \Gamma^d_{ab} + \Gamma^e_{ac}\Gamma^d_{eb} - \Gamma^e_{ab}\Gamma^d_{ec}$
Ricci tensor	$R(X,Y) = \langle f^a, R(e_a, Y)X \rangle$ (f^a is a basis covector; e_a is a basis vector)
(In components)	$R_{ab} = R^d{}_{adb} = \partial_d \Gamma^d_{ab} - \partial_b \Gamma^d_{ad} + \Gamma^e_{ab}\Gamma^d_{ed} - \Gamma^e_{ad}\Gamma^d_{eb} = 2\Gamma^d_{a[b,d]} + 2\Gamma^d_{e[d}\Gamma^e_{b]a}$
Ricci scalar	$R = g^{ab}R_{ab} = R^b{}_b = 2g^{ab}\left(\Gamma^d_{a[b,d]} + \Gamma^d_{e[d}\Gamma^e_{b]a}\right)$
Einstein tensor	$G_{ab} = R_{ab} - \frac{1}{2}R g_{ab}$
Einstein field equations	$G_{ab} = 8\pi T_{ab}$

0 Introduction

The theory of *General Relativity* (GR) is one of the most remarkable scientific achievements in history. Albert Einstein's striking departure from the then-well-established Newtonian theory of gravity was bold (to say the least), and not widely accepted by the physics community at first (contemporaneous physicists were too committed to the idea of the *æther*, a theoretical medium that was assumed to fill the void of space). More than a century has passed since the publication of the theory in 1915 [14], and GR has passed a plethora of rigorous tests, one of the more recent ones being the first direct detection of gravitational waves (GWs) emanating from the inward spiral and merger of a pair of black holes of masses $\sim 36M_{\odot}$ and $\sim 29M_{\odot}$ ($M_{\odot} = 1$ solar mass) [1]. This was a monumental triumph for the theory, worthy of the Nobel Prize in Physics in 2017.

Perhaps the most noteworthy (certainly the most elegant!) aspect of the theory is its simplicity; the *Einstein Field Equations* (EFEs) are a set of ten partial differential equations (PDEs) that can be written in the compact form [1]

$$ {}^{(4)}G^{ab} = 8\pi T^{ab}, \tag{1} $$

where ${}^{(4)}G^{ab}$ is the four-dimensional *Einstein tensor*, which encodes the geometry of spacetime, and T^{ab} is the so-called (four-dimensional) *energy-momentum tensor*, which contains information about the matter/energy content of the system. (In the words of John A. Wheeler, "Spacetime tells matter how to move; matter tells spacetime how to curve.") It is rather remarkable that such a simple-looking expression can be so difficult to solve; even in the absence of matter terms, where ${}^{(4)}G^{ab} = 0$, the calculations required to solve the system (1) are quite daunting. In fact, except for very idealized cases where a number of simplifying symmetries are assumed, we need the full machinery of Numerical Relativity (NR) to tackle the equations. In this report, we shall briefly introduce the basics of NR and then we will investigate the issue of initial data for black holes.

0.1. Motivation

In GR, the evolution of the gravitational field can be posed as an *initial value problem* (or *Cauchy problem*) with constraints (see the original breakthrough paper [15]). In this so-called "3+1 formalism," the EFEs can be determined in two steps:

i) specify the spacetime metric tensor g_{ab} and its time-derivative $\partial_t g_{ab}$ (actually, it will be related quantities) for some initial 3D spacelike hypersurface Σ_0 that has a fixed time coordinate $x^0 = t =$ constant;
ii) provided that we can obtain expressions for second-time derivatives of the 4-metric g_{ab} at all points on the hypersurface from the EFEs, we then integrate forward in time the metric quantities from step i).

[1] We adopt the usual convention in which 4D objects are distinguished from their 3D counterparts by using a superscript (4). There are exceptions to this rule, where 3D objects are denoted by different symbols than their 4D cousins (examples are T_{ab} and g_{ab}, whose 3D counterparts are denoted S_{ab} and γ_{ab}, respectively; these exceptions are merely a matter of convention, of course, but they are widely used in the numerical relativity literature).

However, even though this seems like a straightforward proposal, we immediately face the problem that in GR –unlike in other standard dynamical systems– space and time are two sides of the same coin; these two entities are treated on equal footing. This makes the space-time split that we are so accostumed to seeing in non-relativistic Cauchy problems a much more complicated endeavor. A further complication is the *constraints* of the system; while the system (1) consists of ten coupled PDEs, not all of them are evolution equations:

By the (contracted) *Bianchi identities*,

$$\begin{aligned} 0 &= \nabla_b {}^{(4)}G^{ab} \\ &= \partial_0 {}^{(4)}G^{a0} + \partial_i {}^{(4)}G^{ai} + {}^{(4)}G^{bc}\, {}^{(4)}\Gamma^a{}_{bc} + {}^{(4)}G^{ab}\, {}^{(4)}\Gamma^c{}_{bc}, \end{aligned}$$

we get

$$\partial_t {}^{(4)}G^{a0} = -\partial_i {}^{(4)}G^{ai} - {}^{(4)}G^{bc}\, {}^{(4)}\Gamma^a{}_{bc} - {}^{(4)}G^{ab}\, {}^{(4)}\Gamma^c{}_{bc}. \tag{2}$$

The quantities ${}^{(4)}\Gamma^a{}_{bc}$ are the so-called *Christoffel symbols* (or *connection coefficients*) of the 4-metric g_{ab}. Here (and throughout this paper) we use the convention of identifying the time-component with the zeroth index, as well as the widely adopted Einstein summation convention (refer to the Conventions page for details). Because there is no third-time derivatives (or higher) on the RHS of (2), this implies that there are no second-time derivatives contained in ${}^{(4)}G^{a0}$, and thus the four equations

$${}^{(4)}G^{a0} = 8\pi T^{a0} \tag{3}$$

do not yield any information whatsoever on how the fields evolve in time. Instead, they function as four *constraints* that must be satisfied from the onset on the initial hypersurface at $x^0 = t$ (and remain satisfied throughout the entire evolution!) if we are to have a physically-meaningful system. Thus, we can see that the only true dynamical (*evolution*) equations are encoded in the remaining six field equations

$${}^{(4)}G^{ij} = 8\pi T^{ij}. \tag{4}$$

We will see later on that certain projections of (3) and (4) onto the hypersurfaces will indeed yield the desired constraint and evolution equations of the system.

Whence, according to our discussion above, our first order of business is to somehow find a way to define the role played by space and time, as (somewhat) separate entities. Of course, by this we do not mean “forget about GR and go back to Newtonian/Galilean gravity!” It turns out that there is a special class of spacetimes, known as *globally hyperbolic* spacetimes, that will allow us this sought-after time/space split. First recall that a *Cauchy surface* is a spacelike hypersurface Σ embedded in an ambient manifold $\mathcal{M}$ such that each causal curve without endpoint in $\mathcal{M}$ intersects Σ exactly once. An equivalent way of saying this is that a Cauchy surface for a spacetime $\mathcal{M}$ is an *achronal* subspace $\Sigma \subset M$ (i.e., a subspace Σ in which no two points are timelike-related) which is transversed by every inextendible causal curve in $\mathcal{M}$. Now we properly define the concept of global hyperbolicity:

Definition 1. *A spacetime $\mathcal{M}$ is said to be globally hyperbolic if it admits a Cauchy surface. Equivalently, $\mathcal{M}$ is globally hyperbolic if it satisfies the strongly causal condition (i.e., if every $p \in \mathcal{M}$ has arbitrarily small neighborhoods U in which every every causal curve with endpoints in U is entirely contained in U) and if the “causal diamonds” $J^+(p) \cap J^-(q)$ are compact for all $p, q \in \mathcal{M}$.* [2]

The notion of global hyperbolicity is a crucial feature in Lorentzian geometry that ensures the existence of maximal causal geodesic segments. Physically, this condition is closely connected to the issue of classical determinism and the strong cosmic censorship conjecture [23]. Even though this is by no means a condition satisfied a priori by all spacetimes, the 3+1 formalism assumes that all physically reasonable spacetimes are of this type. This assumption is justified by the desire to have “nice” chronological/causal features in our spacetime (i.e., no *grandfather paradox* or any similar pathological behavior). Moreover, the use of global hyperbolicity allows us to foliate our full 4D spacetime $\mathcal{M}$ in such a way that we can stack 3D spacelike Cauchy slices along a universal time axis, by virtue of $\mathcal{M}$ having topology $\Sigma \times \mathbb{R}$. This is certainly not the only way to foliate $\mathcal{M}$, but it is the most suitable option for the 3+1 formalism.

[2] Here we used standard notation, where $J^+(p) = \{q \in \mathcal{M} \mid p \le q\}$ and $J^-(p) = \{q \in \mathcal{M} \mid q \le p\}$ are the *causal future* and *causal past*, respectively, of $p \in \mathcal{M}$.

Part I

Basics of 3+1 Numerical Relativity

1

The ADM Formalism

Given the foliation of the spacetime manifold granted by the globally hyperbolic condition described in the Introduction (see Fig. 1.1), we can now determine the geometry between two adjacent hypersurfaces Σ_t and $\Sigma_{t+\mathrm{d}t}$ from just three basic ingredients:

I The *3D metric* γ_{ij} (metric induced on Σ: $\gamma_{ab} \equiv \Phi^* g_{ab}$, where $\Phi \colon \Sigma \hookrightarrow \mathcal{M}$ is the embedding of Σ into $\mathcal{M}$) that measures proper distances within the hypersurface itself:

$$dl^2 = \gamma_{ij}\,\mathrm{d}x^i \mathrm{d}x^j.$$

The hypersurface is then said to be

$$\underbrace{\text{– \textit{spacelike}} \iff \gamma_{ab} \text{ is positive definite; i.e., it has signature } (+,+,+);}_{\text{our case}}$$

– *timelike* $\iff$ γ_{ab} is Lorentzian; i.e., it has signature $(-,+,+)$;

– *null* (or *lightlike*) $\iff$ γ_{ab} is degenerate; i.e., it has signature $(0,+,+)$.

(We will shortly justify why we express the spatial metric both as 3D object (γ_{ij}) and a 4D object (γ_{ab}).)

II The *lapse*, α, of proper time (τ) between the hypersurfaces, as measured by *Eulerian* (i.e., *normal*) observers: [1]

$$\mathrm{d}\tau = \alpha(t, x^i)\mathrm{d}t$$

Note that α is sometimes denoted as N by other references, (e.g., [16], [19]).

III The relative velocity β^i between the Eulerian observers:

$$x^i_{t+\mathrm{d}t} = x^i_t - \beta^i(t, x^i)\mathrm{d}t.$$

This 3-vector β^i measures how much the coordinates are shifted as we move from one slice to the next, and it is therefore conventionally named the *shift vector*. (It is also often denoted N^i in the literature.)

As we mentioned earlier, the foliation of $\mathcal{M}$ is not unique and, in fact, neither is the coordinates shift; α determines "how much slicing" is done on $\mathcal{M}$, while β^i dictates how the spatial coordinates change from slice to slice. These quantities are freely-specifiable variables; they encode the gauge freedom that is inherent to a covariant physical theory such as General Relativity.

[1] Such observers have worldlines with tangent vectors that are orthogonal/normal to the spatial hypersurfaces.

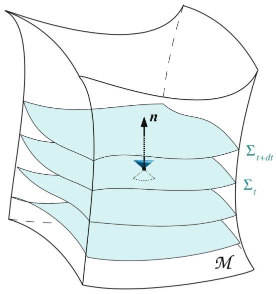


Figure 1.1: Foliation of the spacetime $\mathcal{M}$ by a family of spacelike hypersurfaces $\{\Sigma_t\}_{t\in\mathbb{R}}$. The Σ_t are level surfaces of the (global) coordinate time t, while the normal vector n^a (to be defined later) is orthogonal to these t = constant hypersurfaces. (Image from [16])

From the *universal time function* t (given by the foliation), we have the vector field $\nabla^a t$ that is everywhere normal to the t = constant hypersurface Σ. In fact, $\nabla^a t$ is

- $\underbrace{\text{timelike} \iff \Sigma \text{ is spacelike;}}_{\text{our case}}$
- spacelike $\iff$ Σ is timelike;
- null $\iff$ Σ is null.

We use the 4-metric g_{ab} to normalize $\nabla^a t$:

$$\omega^a = \frac{\nabla^a t}{\|\nabla^a t\|} = \frac{\nabla^a t}{\sqrt{\pm\nabla^a t \nabla_a t}},$$

where the correct sign is

$+$ for a timelike Σ (spacelike $\nabla^a t$);
$-$ $\underbrace{\text{for a spacelike } \Sigma \text{ (timelike } \nabla^a t).}_{\text{our case}}$

Thus, choosing the appropriate sign, we set the lapse function α to be

$$\alpha \equiv (-\nabla^a t \nabla_a t)^{-1/2} \qquad \text{so that} \qquad \omega^a = \alpha \nabla^a t.$$

Then we define the *future-pointing timelike unit normal* n^a to the slice Σ to be [2]

$$n^a \equiv -\omega^a = -\alpha \nabla^a t. \tag{1.1}$$

(We think of n^a as the 4-velocity of an Eulerian observer.) With this defined, we can see that the three scalar quantities that yield the spatial components of the shift vector, β^i, are given by

$$\beta^i = -\alpha\left(\vec{n}\cdot\vec{\nabla}x^i\right). \tag{1.2}$$

These three scalar quantities can then be used to form a full 4-vector β^a (orthogonal to n^a, by construction) which, in the adapted 3+1 coordinates we are about to introduce, will have components $\beta^\mu = (0, \beta^i)$. [3] Equipped with the unit normal and the shift vector, we can also define a *time vector* t^a given by

$$t^a \equiv \alpha n^a + \beta^a, \tag{1.3}$$

which is nothing but the vector tangent to the *time curves*, i.e., the congruence of lines of constant spatial coordinates x^i. This time vector is dual to $\nabla_a t$: for any spatial shift vector β^a,

$$t^a \nabla_a t = (\alpha n^a + \beta^a)\nabla_a t = \underbrace{\alpha n^a \nabla_a t}_{=1} + \underbrace{\beta^a \nabla_a t}_{=0} = 1. \tag{1.4}$$

[2] The minus sign is chosen to ensure that n^a is always future-pointing.
[3] Recall *abstract index notation* (see "Conventions" page for reference).

The relevance of this *duality* will become evident soon. In the *standard 3+1 coordinates*, which we shall present shortly, t^a is our timelike basis vector $e^a_{(0)} = t^a$ (t^a is a natural candidate to be the basis vector $e^a_{(0)}$ precisely because of the duality (1.4)). The remaining three spatial basis vectors $e^a_{(i)}$ are tangent to a particular slice Σ_t (i.e., they satisfy $e^a_{(i)}\nabla_a t = 0$). Moreover, they are *Lie dragged* along t^a,

$$\mathcal{L}_{\vec{t}}\, e^a_{(i)} = 0.$$

We will come back to this in a bit. (Note that some references (e.g., [16]) use a *normal evolution vector* $m^a \equiv \alpha n^a$ in place of t^a to Lie drag the hypersurfaces. This is justified by the fact that m^a is also dual to $\nabla_a t$ (note that in (1.4) the term $\beta^a \nabla_a t$ does not contribute).)

1.1. Projection Operator

We digress for a moment to introduce a crucial object: the *spatial projection operator*

$$P^a{}_b \equiv \delta^a{}_b + n^a n_b. \tag{1.5}$$

This operator projects a 4D tensor onto a spatial slice. For instance, if we take an arbitrary 4-vector v^a, and hit it with the projection operator,

$$\underbrace{v^a}_{\text{arbitrary, 4D}} \xmapsto{P^a{}_b} \underbrace{P^a{}_b v^b}_{\text{purely spatial}}$$

we get a purely spatial object that lies entirely on a hypersurface. We can check that this is indeed the case: first expand $P^a{}_b v^b$,

$$P^a{}_b v^b = (\delta^a{}_b + n^a n_b) v^b = v^a + n^a n_b v^b,$$

and then contract with the normal,

$$\begin{aligned}
(P^a{}_b v^b) n_a &= (v^a + n^a n_b v^b) n_a \\
&= v^a n_a + n^a n_a n_b v^b \\
&= v^a n_a + (-1) v^b n_b && \text{(since } n_a \text{ is normalized and timelike)} \\
&= v^a n_a - v^a n_a = 0. && \text{(relabeling indices)}
\end{aligned}$$

Since there is no contribution whatsoever along n^a, we conclude that $P^a{}_b v^b$ is indeed purely spatial.

In a similar vein, to project higher rank tensors onto a spatial hypersurface, each free index of such tensors is to be contracted with a projection operator (e.g., for a rank-2 tensor T_{ab}, we hit it with two projections, one for each free index: $P_a{}^c P_b{}^d T_{cd}$). Now that this is clear, we see how we get the induced metric (expressed as a full 4D object, γ_{ab}) from the projection of the spacetime metric g_{ab} onto a slice:

$$\gamma_{ab} \equiv P_a{}^c P_b{}^d g_{cd} = \left(\delta^a{}_b + n^a n_b\right)\left(\delta^a{}_b + n^a n_b\right) g_{cd} = g_{ab} + n_a n_b.$$

Thus we have the *spatial metric*

$$\boxed{\gamma_{ab} = g_{ab} + n_a n_b} \tag{1.6}$$

and, similarly, the *inverse spatial metric*,

$$\gamma^{ab} = g^{ac} g^{bd} \gamma_{cd} = g^{ab} + n^a n^b. \tag{1.7}$$

Hence, γ_{ab} is a projection tensor that discards components of 4D geometric objects that lie along n^a; we use it to calculate distances between points that belong to the same spatial hypersurface. We can think of γ_{ab} as first computing four-dimensional distance (with g_{ab}), and then eliminating (with $n_a n_b$) the timelike contribution to the 4D distance calculation. We may check that γ_{ab} is purely spatial by contracting with the normal n^a:

$$n^a \gamma_{ab} = n^a g_{ab} + n^a n_a n_b = n_b - n_b = 0.$$

Now, from (1.6) we see that, if we raise only one index of the spatial metric γ_{ab},

$$\gamma^a{}_b = g^a{}_b + n^a n_b = \delta^a{}_b + n^a n_b,$$

we find out that our projection operator is merely the spatial metric with one raised index

$$P^a{}_b = \gamma^a{}_b.$$

Therefore, from now on we will exclusively use $\gamma^a{}_b$ to denote the *spatial projection operator*; i.e., we rewrite (1.5) as

$$\boxed{\gamma^a{}_b = \delta^a{}_b + n^a n_b.} \tag{1.8}$$

We can now see that the shift vector β^a is nothing but the projection of t^a onto a hypersurface:

$$\gamma^a{}_b t^b = (\delta^a{}_b + n^a n_b)(\alpha n^b + \beta^b) = \alpha\delta^a{}_b n^b + \delta^a{}_b\beta^b + \alpha n^a \underbrace{n_b n^b}_{=-1} + n^a \underbrace{n_b\beta^b}_{=0} = \beta^a. \tag{1.9}$$

This provides us with a coordinate-free expression for the shift vector.

1.2. Coordinate Expressions

We now come back to our discussion of the 3+1 coordinates of the spacetime foliation. We note that, since t^a is aligned with the basis vector $e^a_{(0)}$ (in fact, we *defined* $e^a_{(0)} \equiv t^a$) while all remaining (spatial) coordinates remain constant along t^a, we get the basis components

$$t^\mu = e^\mu_{(0)} = \delta^\mu{}_0 = (1, 0, 0, 0). \tag{1.10}$$

Thus Lie derivatives along the time curves t^a will reduce to ordinary partial derivatives with respect to t; i.e., $\mathcal{L}_{\vec{t}} = \partial_t$ (we will use this later!). Then, as discussed earlier, the remaining three spatial basis vectors $e^a_{(i)}$ reside on a particular slice Σ_t, so that

$$0 = \nabla_a t e^a_{(i)} \overset{\text{by (1.1)}}{=\!=\!=} -\alpha^{-1} n_a e^a_{(i)} \implies n_a e^a_{(i)} = 0.$$

But then, since the $e^a_{(i)}$ are the spatial basis vectors, they must span the hypersurface Σ_t. Hence the condition $n_a e^a_{(i)} = 0$ means that the covariant spatial components of the normal vector must vanish, i.e.,

$$n_i = 0. \tag{1.11}$$

Now, since objects that are purely spatial must vanish (by construction) when contracting with the normal, Eq. (1.11) implies that timelike contravariant components of spatial tensors must vanish. [4] For example, contract the shift vector with the normal,

$$0 \overset{\text{by construction}}{=\!=\!=\!=\!=} n_a\beta^a = n_0\beta^0 + \underbrace{n_i\beta^i}_{=0 \text{ by (1.11)}} = \underbrace{n_0}_{\neq 0}\beta^0 \implies \beta^0 = 0.$$

Combining this with (1.2), we can conclude that, in the adapted coordinates,

$$\beta^\mu = (0, \beta^i), \tag{1.12}$$

as we alluded to earlier. Also, note that from the definition of the time vector (1.3), we have

$$n^a = \frac{t^a}{\alpha} - \frac{\beta^a}{\alpha}.$$

[4] Even though this rationale does not apply to covariant components of spatial tensors (as we can see from (1.13), the contravariant spatial components of the normal are generally nonzero), any contribution along the timelike direction is killed off when contracting with the normal by the condition that $n^{i_k} T_{i_1,\ldots,i_k,\ldots i_n} = 0$ for any purely spatial tensor $T_{i_1,\ldots i_n}$. Therefore *all the information about spatial tensors is effectively contained in their spatial components*. We will use this fact throughout.

Combining this with (1.10) and (1.12), we can get the contravariant components of n^a in the adapted coordinates:

$$n^0 = \alpha^{-1} \underbrace{t^0}_{=1} - \alpha^{-1} \underbrace{\beta^0}_{=0} = \alpha^{-1},$$

while

$$n^i = \alpha^{-1} \underbrace{t^i}_{0} - \alpha^{-1}\beta^i = -\alpha^{-1}\beta^i.$$

Thus we have found

$$n^\mu = (\alpha^{-1}, -\alpha^{-1}\beta^i), \tag{1.13}$$

and since n^a is unit timelike,

$$-1 = n^a n_a \overset{\text{by (1.11)}}{=\!=\!=} n^0 n_0 \implies n_0 = -\frac{1}{n^0} = -\alpha.$$

Hence, combining this with (1.11), we have all covariant components of the normal in the adapted coordinates

$$n_\mu = (-\alpha, 0, 0, 0). \tag{1.14}$$

Now, from (1.6),

$$\gamma_{ij} = g_{ij} + \underbrace{n_i n_j}_{=0} = g_{ij}, \tag{1.15}$$

so that the spatial metric on Σ is just the spatial part of the spacetime 4-metric g_{ab}. Note also that, even though the covariant components do not necessarily vanish ($\gamma_{0\mu} = g_{0\mu} + n_0 n_\mu = g_{0\mu} + n_0 n_0 = g_{0\mu} + \alpha^2 \neq 0$, in general), any contribution to the timelike direction can be safely ignored since $n^a \gamma_{ab} = 0$ (see footnote 4). On the other hand, timelike components of spatial contravariant tensors do vanish (see discussion below equation (1.11)), so we must have $\gamma^{a0} = 0$. Therefore, from (1.7), we get the components of the inverse spacetime metric in these adapted coordinates:

$$\begin{aligned}
g^{ab} &= \gamma^{ab} - n^a n^b \\
g^{0a} &= -n^0 n^a \implies g^{00} = -\alpha^{-2} \quad \& \quad g^{0i} = \alpha^{-2}\beta^i \\
g^{ij} &= \gamma^{ij} - n^i n^j = \gamma^{ij} - (-\alpha^{-1}\beta^i)(-\alpha^{-1}\beta^j) = \gamma^{ij} - \alpha^{-2}\beta^i\beta^j.
\end{aligned}$$

In matrix form,

$$g^{\mu\nu} = \begin{pmatrix} -1/\alpha^2 & \beta^i/\alpha^2 \\ \beta^j/\alpha^2 & \gamma^{ij} - \beta^i\beta^j/\alpha^2 \end{pmatrix}. \tag{1.16}$$

Now, by the condition $g^{ab} g_{bc} = \delta^a{}_c$, we can invert (1.16) to write the spacetime metric in 3+1 coordinates:

$$g_{\mu\nu} = \begin{pmatrix} -\alpha^2 + \beta_k\beta^k & \beta_i \\ \beta_j & \gamma_{ij} \end{pmatrix}. \tag{1.17}$$

The covariant components β_i shown above come from lowering with the spatial metric, i.e., $\beta_i = \gamma_{ik}\beta^k$. We will always use the spatial metric to raise/lower indices of spatial objects, because γ_{ij} and γ^{ij} are inverses of each other in the adapted coordinates:

$$\begin{aligned}
\gamma^{ik}\gamma_{kj} &= (g^{ik} + n^i n^k)(g_{kj} + n_k n_j) \\
&= g^{ik} g_{kj} + g^{ik} n_k n_j + n^i n^k g_{kj} + n^i n^k n_k n_j \\
&= \delta^i{}_j + n^i \underbrace{n_j}_{=0} + n^i \underbrace{n_j}_{=0} - n^i \underbrace{n_j}_{=0} = \delta^i{}_j.
\end{aligned}$$

From (1.17) we see that the *line element* of the full spacetime metric in 3+1 coordinates is given by

$$\boxed{ds^2 = \left(-\alpha^2 + \beta_i\beta^i\right) \mathrm{d}t^2 + 2\beta_i \, \mathrm{d}t \mathrm{d}x^i + \gamma_{ij} \, \mathrm{d}x^i \mathrm{d}x^j.} \tag{1.18}$$

1.3. 3D Curvature

As we saw in the Introduction, the EFEs (c.f., Eq. (1)) relate contractions of the 4D Riemann tensor (namely, the *Ricci tensor* and the *Ricci scalar*) to the energy-momentum tensor (these contractions are encoded in the Einstein tensor ${}^{(4)}G_{ab}$). However, given our interest in the 3+1 formalism, we need to find a way to translate these four-dimensional (*spacetime*) quantities into three-dimensional (*spatial*) objects. As the reader may have wisely guessed, the projection operator (1.8) will play a key role in accomplishing this task. These projections will allow us to distinguish between properties that are *intrinsic* to the 3D geometry from those that are *extrinsic* (i.e., that depend on the embedding into the ambient 4D manifold). To elaborate further, we start with the following crucial definition:

Definition 2. *The* spatial connection D *intrinsic to a hypersurface* Σ *satisfies the following: Let* $\vec{X}, \vec{Y}_{(a)} \in \mathfrak{X}(\Sigma)$ *be vector fields on* Σ *(sections of the* tangent bundle $\Sigma \to T\Sigma$*) and let* $\widetilde{\omega}^{(a)} \in \mathfrak{X}^*(\Sigma)$ *be* 1*-forms on* Σ *(sections of the* cotangent bundle $\Sigma \to T^*\Sigma$*). Then for any* $\binom{a}{b}$ *tensor field* $\boldsymbol{T} \in \mathcal{T}_b{}^a(\Sigma)$*, the map*

$$D\boldsymbol{T}: \underbrace{\mathfrak{X}^*(\Sigma) \times \ldots \times \mathfrak{X}^*(\Sigma)}_{a \text{ times}} \times \underbrace{\mathfrak{X}(\Sigma) \times \ldots \times \mathfrak{X}(\Sigma)}_{b+1 \text{ times}} \to C^\infty(\Sigma)$$

given by

$$D\boldsymbol{T}(\widetilde{\omega}^1, \ldots, \widetilde{\omega}^a, \vec{Y}_1, \ldots, \vec{Y}_b, \vec{X}) = D_{\vec{X}}\boldsymbol{T}(\widetilde{\omega}^1, \ldots, \widetilde{\omega}^a, \vec{Y}_1, \ldots, \vec{Y}_b)$$

defines an $\binom{a}{b+1}$ *tensor field, which we will call the* spatial covariant derivative*. It can be shown also that* D *is torsion-free and compatible with the 3D metric, i.e.,* $D_c\gamma_{ab} = 0$*.*

In a coordinate chart,

$$\begin{aligned}(D\boldsymbol{T})^{i_1\ldots i_a}{}_{j_1\ldots j_b c} &= D_c T^{i_1\ldots i_a}{}_{j_1\ldots j_b} \\ &= \partial_c T^{i_1\ldots i_a}{}_{j_1\ldots j_b} + \sum_{d=1}^{a} T^{i_1\ldots e\ldots i_a}{}_{j_1\ldots j_b}\,\Gamma^{i_d}_{ec} - \sum_{d=1}^{b} T^{i_1\ldots i_a}{}_{j_1\ldots e\ldots j_b}\,\Gamma^{e}_{j_d c},\end{aligned} \tag{1.19}$$

where

$$\Gamma^a_{bc} = \frac{1}{2}\gamma^{ad}(\partial_c\gamma_{db} + \partial_b\gamma_{dc} - \partial_d\gamma_{bc}). \tag{1.20}$$

For instance, take a $\binom{1}{1}$ tensor field $T^a{}_b$; then its covariant spatial derivative with respect to the $\vec{e}_{(c)}$ basis vector (i.e., the geometric object that shows how much $T^a{}_b$ varies as it is transported along congruence lines of $\vec{e}_{(c)}$) is the $\binom{1}{2}$ tensor field given by

$$(D\boldsymbol{T})^a{}_{bc} = T^a{}_{b;c} = D_c T^a{}_b = \partial_c T^a{}_b + T^d{}_b\,\Gamma^a_{dc} - T^a{}_d\,\Gamma^d_{bc}.$$

(The semicolon notation is commonly used in the GR literature to denote covariant differentiation. Instead, a comma is used for the standard partial derivative in flat space; e.g., $T^a{}_{b,c} \equiv \partial_c T^a{}_b$.) Having defined the above, it is not hard to show that the spatial covariant derivative is furnished by projecting *all* indices present in a 4D covariant derivative ∇ (connection of the ambient manifold $\mathcal{M}$) onto Σ; that is,

$$D_a T^{i_1\ldots i_b}{}_{j_1\ldots j_c} = \gamma_a{}^d\gamma^{i_1}{}_{k_1}\ldots\gamma^{i_b}{}_{k_b}\gamma_{j_1}{}^{\ell_1}\ldots\gamma_{j_c}{}^{\ell_c}\,\nabla_d T^{k_1\ldots k_b}{}_{\ell_1\ldots\ell_c}. \tag{1.21}$$

For a simple example, consider again a $\binom{1}{1}$ tensor field $T^a{}_b$. Then,

$$D_a T^b{}_c = \gamma_a{}^d\gamma^b{}_e\gamma_c{}^f\nabla_d T^e{}_f.$$

Now equipped with the spatial covariant derivative, we define the *3D Riemann tensor* $R^d{}_{abc}$ associated with γ_{ab} by requiring the following two properties:

⋇ (Ricci identity) for any spatial vector v^a,

$$2D_{[a}D_{b]}v^c = R^c{}_{dab}v^d; \tag{1.22}$$

⋇ (Purely spatial tensor) the contraction with the normal vanishes

$$R^d{}_{cba}n_d = 0. \tag{1.23}$$

The brackets used on the indices in Eq. (1.22) are common notation in GR; they are used to denote the *antisymmetric* part of a tensor $\boldsymbol{T}$:

$$T_{[\mu_1\ldots\mu_k]} = \frac{1}{k!}\hat{\epsilon}^{\mu_1\ldots\mu_k}T_{\mu_1\ldots\mu_k}, \tag{1.24}$$

where the *Levi-Civita symbol* $\hat{\epsilon}$ is given by

$$\hat{\epsilon}^{\mu_1\ldots\mu_k} = \begin{cases} +1 & \text{if } (\mu_1\ldots\mu_k) \text{ is an even permutation of } 1,\ldots,k; \\ -1 & \text{if } (\mu_1\ldots\mu_k) \text{ is an odd permutation of } 1,\ldots,k; \\ 0 & \text{if there are any repeated indices in } 1,\ldots,k. \end{cases}$$

Similarly, to denote the *symmetric* part of a tensor $\boldsymbol{T}$ we use parentheses on the indices:

$$T_{(\mu_1\ldots\mu_k)} = \frac{1}{k!}\hat{\sigma}^{\mu_1\ldots\mu_k}T_{\mu_1\ldots\mu_k}, \tag{1.25}$$

where $\hat{\sigma}$ is given by

$$\hat{\sigma}^{\mu_1\ldots\mu_k} = \begin{cases} +1 & \text{for any permutation } (\mu_1\ldots\mu_k) \text{ of } 1,\ldots,k; \\ 0 & \text{if there are any repeated indices in } 1,\ldots,k. \end{cases}$$

For example,

$$\begin{aligned} T_{[ab]} &= \frac{1}{2}(T_{ab} - T_{ba}) \\ T_{(ab)} &= \frac{1}{2}(T_{ab} + T_{ba}) \\ T_{[abc]} &= \frac{1}{3!}(T_{abc} + T_{bca} + T_{cab} - T_{acb} - T_{cba} - T_{bac}) \\ T_{(abc)} &= \frac{1}{3!}(T_{abc} + T_{bca} + T_{cab} + T_{acb} + T_{cba} + T_{bac}). \end{aligned}$$

Now back to the topic at hand. It is not hard to show that, in a coordinate basis, the Riemann tensor takes the form

$$R^d{}_{abc} = \partial_b\Gamma^d_{ac} - \partial_c\Gamma^d_{ab} + \Gamma^e_{ac}\Gamma^d_{eb} - \Gamma^e_{ab}\Gamma^d_{ec}, \tag{1.26}$$

where the Christoffel symbols Γ^c_{ab} are the connection coefficients of the spatial metric (c.f., Eq. (1.20)). Moreover, a contraction of Eq. (1.26) yields the *3D Ricci tensor*

$$\begin{aligned} R_{ab} = R^d{}_{adb} &= \partial_d\Gamma^d_{ab} - \partial_b\Gamma^d_{ad} + \Gamma^e_{ab}\Gamma^d_{ed} - \Gamma^e_{ad}\Gamma^d_{eb} \\ &= 2\Gamma^d_{a[b,d]} + 2\Gamma^d_{e[d}\Gamma^e_{b]a}, \end{aligned} \tag{1.27}$$

and yet a further contraction provides the *3D Ricci scalar*:

$$R = R^a{}_a = \gamma^{ab}R_{ab} = 2\gamma^{ab}\left(\Gamma^d_{a[b,d]} + \Gamma^d_{e[d}\Gamma^e_{b]a}\right). \tag{1.28}$$

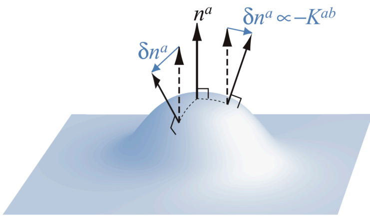


Figure 1.2: K_{ab} yields information about the bending of the slice in the ambient spacetime by measuring how much the normal varies from point to point on said slice; i.e., it measures the change of the normal vector under parallel transport within a slice. (Image from [6])

The 3D Riemann tensor (and its contractions) encode information about the geometry that is intrinsic to the hypersurfaces. These quantities are always well defined, and they do not depend on the notion of an embedding into some higher-dimensional object. On the other hand, we do know that these surfaces *are* embedded in an ambient four-dimensional spacetime manifold. Furthermore, based on our discussions of the 3+1 formalism thus far, we also know that we need to find a way to relate spacetime 4D objects to spatial ones. In particular, we would like to have a sense of how the geometry pertaining to the slices is related to the ambient 4D geometry. To that end, we now define a crucial object: the *extrinsic curvature tensor*, which is given by [5]

$$\boxed{K_{ab} = -\gamma_a{}^c \gamma_b{}^d \nabla_c n_d.} \tag{1.29}$$

This quantity measures how much n^a varies as we move from point to point on a particular slice Σ, and in doing so it describes how the geometry of Σ is embedded in $\mathcal{M}$ (see Fig. 1.2). Let us now expand:

$$\begin{aligned} K_{ab} &= -\gamma_a{}^c \gamma_b{}^d \nabla_c n_d \\ &= -\left[(\delta_a{}^c + n_a n^c)(\delta_b{}^d + n_b n^d)\nabla_c n_d\right] \\ &= -\left[(\delta_a{}^c \delta_b{}^d + n_a n^c \delta_b{}^d + \delta_a{}^c n_b n^d + n_a n^c n_b n^d)\nabla_c n_d\right] \\ &= -[\nabla_a n_b + n_a n^c \nabla_c n_b + n_b \underbrace{n^d \nabla_a n_d}_{=0} + n_a n_b n^c \underbrace{n^d \nabla_c n_d}_{=0}] \\ &= -\nabla_a n_b - n_a n^c \nabla_c n_b. \end{aligned}$$

On the fourth equality we claimed that $n^d \nabla_a n_d = 0$ from the the following fact:

$$\begin{aligned} \underbrace{\nabla_a(\overbrace{n_b n^b}^{=-1})}_{=0} &= n^b \nabla_a n_b + n_b \nabla_a n^b \\ \implies 0 &= n^b \nabla_a n_b + \underbrace{n_b \nabla_a g^{bc} n_c}_{=n_b g^{bc} \nabla_a n_c = n^c \nabla_a n_c} \\ \implies n^b \nabla_a n_b &= -n^b \nabla_a n_b \\ \implies n^b \nabla_a n_b &= 0. \end{aligned}$$

Hence, once we expand (1.29) we have

$$\boxed{K_{ab} = -\nabla_a n_b - n_a n^c \nabla_c n_b.} \tag{1.30}$$

This form is more practical for computations, so it shall be the one we use hereafter (along with Eq. (1.34); see below). Note that, since n^a is regarded as the 4-velocity of some Eulerian observer, we may consider the quantity $n^c \nabla_c n_b$ to be the *4-acceleration* a_b of such Eulerian observer:

$$\mathsf{a}_b \equiv n^c \nabla_c n_b. \tag{1.31}$$

[5] The minus sign is merely a convention in the NR community.

Now expand (1.31):

$$
\begin{aligned}
\mathsf{a}_a &= n^b\nabla_b n_a = n^b\nabla_b \underbrace{(-\alpha\nabla_a t)}_{\text{def of } n_a} = -n^b\nabla_b\alpha \underbrace{\nabla_a t}_{=-\frac{1}{\alpha}n_a} - \alpha n^b \underbrace{\nabla_b\nabla_a t}_{=\nabla_a\nabla_b t} \\
&= \frac{1}{\alpha}n_a n^b\nabla_b\alpha - \alpha n^b\nabla_a\left(-\frac{1}{\alpha}n_b\right) \\
&= \frac{1}{\alpha}n_a n^b\nabla_b\alpha + \alpha\frac{1}{\alpha}\underbrace{n^b\nabla_a n_b}_{=0} + \alpha\underbrace{n^b n_b}_{=-1}\underbrace{\nabla_a\frac{1}{\alpha}}_{=-\alpha^{-2}\nabla_a\alpha} \\
&= \frac{1}{\alpha}n_a n^b\nabla_b\alpha - \alpha\left(-\frac{1}{\alpha^2}\nabla_a\alpha\right) = \frac{1}{\alpha}\left(n_a n^b\nabla_b\alpha + \nabla_a\alpha\right) \\
&= \frac{1}{\alpha}\left((\delta_a{}^b + n_a n^b)\nabla_b\alpha\right) = \frac{1}{\alpha}\gamma_a{}^b\nabla_b\alpha = \frac{1}{\alpha}D_a\alpha \\
&= D_a\log\alpha.
\end{aligned}
$$

This shows that a_b is actually the spatial gradient of the logarithm of the lapse function:

$$\boxed{\mathsf{a}_a = D_a\log\alpha.} \tag{1.32}$$

Now, since it will come in handy later, we take yet another spatial derivate of this quantity:

$$
\begin{aligned}
D_a\mathsf{a}_b &= D_a D_b\log\alpha \\
&= D_a\left(\frac{1}{\alpha}D_b\alpha\right) = \frac{1}{\alpha}D_a D_b\alpha + D_a\left(\frac{1}{\alpha}\right)D_b\alpha \\
&= \frac{1}{\alpha}D_a D_b\alpha - \frac{1}{\alpha^2}D_a\alpha\, D_b\alpha = \frac{1}{\alpha}D_a D_b\alpha - \underbrace{\frac{1}{\alpha}D_a\alpha}_{=D_a\log\alpha}\;\underbrace{\frac{1}{\alpha}D_b\alpha}_{=D_b\log\alpha} \\
&= \frac{1}{\alpha}D_a D_b\alpha - \mathsf{a}_a\mathsf{a}_b.
\end{aligned} \tag{1.33}
$$

We will use both(1.32) and (1.33) later when computing a certain projection of the 4D Riemann tensor.

It is important to make sure that K_{ab} is indeed a purely spatial object:

$$
\begin{aligned}
n^a K_{ab} &= n^a(-\nabla_a n_b - n_a n^c\nabla_c n_b) \\
&= -n^a\nabla_a n_b - n^a n_a n^c\nabla_c n_b \\
&= -n^a\nabla_a n_b + n^a\nabla_a n_b = 0. \qquad \text{(after relabeling)}
\end{aligned}
$$

This is reassuring. It allows us us to discard timelike components (we discussed this earlier) and focus exclusively on the spatial components K_{ij} (we will certainly use this fact later). Another key property of K_{ab} is its symmetry ($K_{ab} = K_{ba}$); we prove this by writing it as the *Lie derivative* of the spatial metric along the normal direction: [6]

$$\boxed{K_{ab} = -\frac{1}{2}\mathcal{L}_{\vec{n}}\gamma_{ab}.} \tag{1.34}$$

Proof. We expand using the definition of the Lie derivative:

$$
\begin{aligned}
\mathcal{L}_{\vec{n}}\gamma_{ab} &= n^c\nabla_c\gamma_{ab} + \gamma_{ac}\nabla_b n^c + \gamma_{cb}\nabla_a n^c \\
&= n^c\nabla_c(n_a n_b) + g_{ac}\nabla_b n^c + g_{cb}\nabla_a n^c \\
&= n^c n_a\nabla_c n_b + n^c n_b\nabla_c n_a + \nabla_b n_a + \nabla_a n_b \\
&= (\gamma_a{}^c - g_a{}^c)\nabla_c n_b + (\gamma_b{}^c - g_b{}^c)\nabla_c n_a + \nabla_b n_a + \nabla_a n_b \\
&= \gamma_a{}^c\nabla_c n_b + \gamma_b{}^c\nabla_c n_a = -2K_{ab}.
\end{aligned}
$$

♠

[6] This is in fact taken as the definition of K_{ab} in many references!

Here we used the fact that $\nabla_c g_{ab} = 0$ and the identity $n^c \nabla_a n_c = 0$. Another (more compact) computation shows the same result:

$$\begin{aligned}\mathcal{L}_{\vec{n}}\gamma_{ab} &= \mathcal{L}_{\vec{n}}(g_{ab} + n_a n_b) = 2\nabla_{(a}n_{b)} + n_a\mathcal{L}_{\vec{n}}n_b + n_b\mathcal{L}_{\vec{n}}n_a \\ &= 2\left(\nabla_{(a}n_{b)} + n_{(a}\mathrm{a}_{b)}\right) = -2K_{ab}.\end{aligned}$$

Since n^a is a timelike vector, equation (1.34) illustrates the intuitive interpretation of the extrinsic curvature as a geometric generalization of the "time derivative" of the spatial metric γ_{ab}, i.e., the "velocity" of the spatial metric as seen by the Eulerian observers. However, $\mathcal{L}_{\vec{n}}$ is not a natural time derivative, since n^a is not dual to the surface 1-form $\nabla_a t = \nabla_a t$, i.e., their dot product is not unity:

$$n^a\nabla_a t = -\alpha\underbrace{\nabla^a t\nabla_a t}_{=-\alpha^{-2}} = \alpha^{-1}.$$

Instead, recall that the time vector $t^a = \alpha n^a + \beta^a$ *is* in fact dual to $\nabla_a t$, as we showed via equation (1.4). Thus we can use t^a to rewrite (1.34) as a more natural time derivative of the metric:

$$\begin{aligned}K_{ab} = -\frac{1}{2}\mathcal{L}_{\vec{n}}\gamma_{ab} &= -\frac{1}{2}\mathcal{L}_{\frac{\vec{t}-\vec{\beta}}{\alpha}}\gamma_{ab} \\ &= -\frac{1}{2\alpha}\left(\mathcal{L}_{\vec{t}}\gamma_{ab} - \mathcal{L}_{\vec{\beta}}\gamma_{ab}\right) \\ &= -\frac{1}{2\alpha}\left(\partial_t\gamma_{ab} - \mathcal{L}_{\vec{\beta}}\gamma_{ab}\right),\end{aligned} \qquad (1.35)$$

where on the last line we used the fact that, in the adapted coordinates, $\mathcal{L}_{\vec{t}}$ reduces to ∂_t.

1.4. ADM Evolution & Constraints

The twelve quantities $\{\gamma_{ij}, K_{ij}\}$ encode all the geometric data, both intrinsic and extrinsic, of the 3D hypersurfaces. Thus, in our efforts to pose the EFEs as a Cauchy problem we need to determine the evolution of this system (c.f., Eq. (4)), starting with some initial data $\{\gamma_{ij}^{(0)}, K_{ij}^{(0)}\}$ that is prescribed on an initial slice $\Sigma_{t=0}$. However, we recall that this data cannot be arbitrary, as constraints must be satisfied at the initial slice *and* throughout the entire time-evolution (c.f., Eq. (3)). In this section we derive both the evolution and constraint equations, in the ADM formalism. A conformal reformulation of these equations will be presented in the next chapter, when we discuss the so-called *BSSN* formalism.

Let us start by rewriting Eq. (1.35) as

$$\partial_t\gamma_{ab} = \mathcal{L}_{\vec{\beta}}\gamma_{ab} - 2\alpha K_{ab}. \qquad (1.36)$$

Since –as we have previously discussed– the entire content of any spatial tensor is available from its spatial components alone, we can drop the timelike components and expand:

$$\begin{aligned}\partial_t\gamma_{ij} &= \mathcal{L}_{\vec{\beta}}\gamma_{ij} - 2\alpha K_{ij} \\ &= \beta^k\underbrace{D_k\gamma_{ij}}_{=0} + D_i(\gamma_{kj}\beta^k) + D_j(\gamma_{ik}\beta^k) - 2\alpha K_{ij} \\ &= D_i\beta_j + D_j\beta_i - 2\alpha K_{ij}.\end{aligned}$$

Hence, (1.36) boils down to

$$\boxed{\partial_t\gamma_{ij} = 2D_{(i}\beta_{j)} - 2\alpha K_{ij}.} \qquad (1.37)$$

This is our sought-after *evolution equation of the spatial metric*. While we are at it, let us also present a useful contraction of this equation that will come in handy later. Per usual convention, we denote the determinant of the spatial metric by $\gamma \equiv \det\gamma_{ij}$. Then,

$$\begin{aligned}
\partial_t \log \sqrt{\gamma} = \frac{1}{2}\partial_t \log \gamma = \frac{1}{2}\frac{1}{\gamma}\partial_t \gamma \\
&= \frac{1}{2}\mathrm{Tr}\left(\gamma^{ij}\partial_t \gamma_{kl}\right) \\
&= \frac{1}{2}\gamma^{ij}\partial_t \gamma_{ij} \\
&= \frac{1}{2}\gamma^{ij}\left(-2\alpha K_{ij} + D_i\beta_j + D_j\beta_i\right) && \text{(By (1.37))} \\
&= -\alpha K + D_i \beta^i. && (1.38)
\end{aligned}$$

Here we used *Jacobi's formula*: For an invertible matrix A,

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\det A(t)\right] = \det A(t) \cdot \mathrm{Tr}\left[A^{-1}(t) \cdot \frac{\mathrm{d}}{\mathrm{d}t}A(t)\right]. \tag{1.39}$$

We note that to derive the evolution of the spatial metric we did not use the EFEs at all. That all changes for the derivation of the evolution of the extrinsic curvature –as well as for the constraints.– Our starting point is to cast the EFEs in 3+1 form, which can be achieved by contracting them with the projection operator $\gamma^a{}_b$ and with the normal vector n^a. There are only three unique types of contractions (all other projections vanish identically thanks to the symmetries of the Riemann tensor):

- ⋇ Normal projection (1 equation):

$$n^a n^b \left({}^{(4)}G_{ab} - 8\pi T_{ab}\right) = 0. \tag{1.40}$$

- ⋇ Projection onto the hypersurface (6 equations):

$$\gamma_c{}^a \gamma_d{}^b \left({}^{(4)}G_{ab} - 8\pi T_{ab}\right) = 0. \tag{1.41}$$

- ⋇ Mixed projection (3 equations):

$$\gamma_c{}^b \left[n^a \left({}^{(4)}G_{ab} - 8\pi T_{ab}\right)\right] = 0. \tag{1.42}$$

These expressions come about by using the celebrated *Gauss-Codazzi*, *Codazzi-Mainardi*, and *Ricci* equations, which are given, respectively, by the following:

$$\boxed{\begin{aligned}
\gamma_a{}^e \gamma_b{}^f \gamma_c{}^g \gamma_d{}^h \, {}^{(4)}R_{efgh} &= R_{abcd} + K_{ac}K_{bd} - K_{ad}K_{cb} \\
\gamma_a{}^e \gamma_b{}^f \gamma_c{}^g n^h \, {}^{(4)}R_{efgh} &= D_b K_{ac} - D_a K_{bc} \\
\gamma_a{}^q \gamma_b{}^r n^c n^d \, {}^{(4)}R_{qcrd} &= \mathcal{L}_{\vec{n}} K_{ab} + \frac{1}{\alpha} D_a D_b \alpha + K_b{}^c K_{ac}.
\end{aligned}}
\begin{aligned} &(1.43a) \\ &(1.43b) \\ &(1.43c) \end{aligned}$$

These three important equations are proven in gory detail in Appendix A. Note how Eqs. (1.43a) and (1.43b) depend exclusively on the spatial metric, the extrinsic curvature, and their spatial derivatives; they will give rise to the constraint equations. On the other hand, Eq. (1.43c) will yield the *evolution equation for the extrinsic curvature*, which we will show last.

Without further ado then, let us now derive the constraint equations from contractions of (1.43a) and (1.43b). Starting with (1.43a), first raise an index and then contract (all with the 3-metric γ_{ab}):

$$\begin{aligned}
\gamma^{pa}\gamma_a{}^e \gamma_b{}^f \gamma_c{}^g \gamma_d{}^h \, {}^{(4)}R_{efgh} &= \gamma^{pa}R_{abcd} + \gamma^{pa}K_{ac}K_{bd} - \gamma^{pa}K_{ad}K_{cb} \\
\gamma^{pe}\gamma_b{}^f \gamma_c{}^g \gamma_d{}^h \, {}^{(4)}R_{efgh} &= R^p{}_{bcd} + K^p{}_c K_{bd} - K^p{}_d K_{cb} \\
\gamma_b{}^f \gamma_d{}^h \gamma^{eg} \, {}^{(4)}R_{efgh} &= R_{bd} + K K_{bd} - K^c{}_d K_{cb}, && (1.44)
\end{aligned}$$

where on the third line we contracted on indices p and c, and we introduced the *trace of the extrinsic curvature* $K \equiv K^a{}_a$. Now, a further contraction yields

$$\begin{aligned}
\gamma^{pb}\gamma_b{}^f\gamma_d{}^h\gamma^{eg\,(4)}R_{efgh} &= \gamma^{pb}R_{bd} + \gamma^{pb}KK_{bd} - \gamma^{pb}K^c{}_dK_{cb} \\
\gamma^{pf}\gamma^{eg}\gamma_d{}^{h\,(4)}R_{efgh} &= R^p{}_d + KK^p{}_d - K^c{}_dK_c{}^p \\
\gamma^{fh}\gamma^{eg\,(4)}R_{efgh} &= R + K^2 - K^c{}_pK_c{}^p. \qquad (1.45)
\end{aligned}$$

Here we again contracted on indices p and d on the last line. Now note that

$$K^c{}_pK_c{}^p = K^c{}_p\gamma^{pr}K_{cr} = K^{cr}K_{cr},$$

and we can also expand on the left hand side of (1.45) as

$$\begin{aligned}
\gamma^{fh}\gamma^{eg\,(4)}R_{efgh} &= (g^{fh} + n^fn^h)(g^{eg} + n^en^g)\,^{(4)}R_{efgh} \\
&= (g^{fh}g^{eg} + n^fn^hg^{eg} + n^en^gg^{fh} + n^fn^hn^en^g)\,^{(4)}R_{efgh} \\
&= g^{fh}g^{eg\,(4)}R_{efgh} + n^fn^hg^{eg\,(4)}R_{efgh} + n^en^gg^{fh\,(4)}R_{fehg} \\
&\quad + \underbrace{n^fn^hn^en^{g\,(4)}R_{efgh}}_{=0 \text{ by symmetries of } ^{(4)}R_{efgh}} \\
&= g^{fh\,(4)}R_{fh} + n^fn^{h\,(4)}R_{fh} + n^en^{g\,(4)}R_{eg} \\
&= {}^{(4)}R + 2n^fn^{h\,(4)}R_{fh}. \qquad \text{(by relabeling)}
\end{aligned}$$

Thus we can rewrite (1.45) as

$$^{(4)}R + 2n^an^{b\,(4)}R_{ab} = R + K^2 - K^{ab}K_{ab}.$$

Yet we can do better…Close inspection of the left hand side tells us that the Einstein tensor is lurking somewhere:

$$\begin{aligned}
^{(4)}R + 2n^an^{b\,(4)}R_{ab} &= -\underbrace{n^an_a}_{\text{since } n^an_a = -1}\,^{(4)}R + 2n^an^{b\,(4)}R_{ab} \\
&= -g_{ab}n^an^{b\,(4)}R + 2n^an^{b\,(4)}R_{ab} \\
&= 2n^an^b\left(^{(4)}R_{ab} - \frac{1}{2}\,^{(4)}Rg_{ab}\right) \\
&= 2n^an^{b\,(4)}G_{ab}.
\end{aligned}$$

Then, by means of the EFEs, $^{(4)}G_{ab} = 8\pi T_{ab}$, we get

$$\begin{aligned}
R + K^2 - K^{ab}K_{ab} &= 2n^an^{b\,(4)}G_{ab} \\
R + K^2 - K^{ab}K_{ab} &= 16\pi n^an^bT_{ab}.
\end{aligned}$$

Defining the total *energy density* ρ (as measured by a normal observer n^a) as

$$\rho \equiv n^an^bT_{ab}, \qquad (1.46)$$

we end up with

$$R + K^2 - K^{ab}K_{ab} = 16\pi\rho. \qquad (1.47)$$

This is the so-called *Hamiltonian constraint* which, after dropping timelike components, we write as

$$\boxed{R + K^2 - K^{ij}K_{ij} = 16\pi\rho.} \qquad (1.48)$$

Now on to find the remaining constraint equation; we use (1.43b), raise an index and then contract (all with the 3-metric γ_{ab}):

$$\begin{aligned}
\gamma^{rc}\gamma_a{}^d\gamma_b{}^e\gamma_c{}^f n^p\,{}^{(4)}R_{defp} &= \gamma^{rc}D_bK_{ac} - \gamma^{rc}D_aK_{bc} \\
\gamma_a{}^d\gamma_b{}^e\gamma^{rf} n^p\,{}^{(4)}R_{defp} &= D_bK_a{}^r - D_aK_b{}^r && \text{(Since } D_a \text{ is compatible with } \gamma_{ab}\text{)} \\
\gamma_a{}^d\gamma^{ef} n^p\,{}^{(4)}R_{defp} &= D_bK_a{}^b - D_aK, && (1.49)
\end{aligned}$$

where on the last line we contracted on indices r and b. Then expanding the left hand side of (1.49)

$$\begin{aligned}
\gamma_a{}^d\gamma^{ef} n^p\,{}^{(4)}R_{defp} &= \gamma_a{}^d\left(g^{ef} + n^e n^f\right) n^p\,{}^{(4)}R_{defp} \\
&= \gamma_a{}^d n^p g^{ef}\,{}^{(4)}R_{defp} + \gamma_a{}^d \underbrace{n^e n^f n^p\,{}^{(4)}R_{defp}}_{=0 \text{ by symmetries of } {}^{(4)}R_{abcd}} \\
&= -\gamma_a{}^d n^p g^{ef}\,{}^{(4)}R_{edfp} = -\gamma_a{}^d n^p\,{}^{(4)}R_{dp}.
\end{aligned}$$

So, plugging back into (1.49), we get

$$D_bK_a{}^b - D_aK = -\gamma_a{}^d n^p\,{}^{(4)}R_{dp}. \tag{1.50}$$

Yet we want to bring in the Einstein tensor to the scene, so we can push a bit further and expand the right hand side of (1.50):

$$-\gamma_a{}^d n^p\,{}^{(4)}R_{dp} = -(\gamma_a{}^d n^p\,{}^{(4)}R_{dp} - \frac{1}{2}\underbrace{\gamma_a{}^d n^p g_{dp}}_{=\gamma_{ap}n^p=0}\,{}^{(4)}R) = -\gamma_a{}^d n^p\,{}^{(4)}G_{dp}.$$

Then, once again invoking the EFEs, ${}^{(4)}G_{ab} = 8\pi T_{ab}$, we get

$$\begin{aligned}
D_bK_a{}^b - D_aK &= -\gamma_a{}^d n^p\,{}^{(4)}G_{dp} \\
D_bK_a{}^b - D_aK &= -\gamma_a{}^d n^p 8\pi T_{dp}\,.
\end{aligned}$$

Defining the *momentum density* S_a (as measured by a normal observer n^a) by

$$S_a \equiv -\gamma_a{}^b n^c T_{bc}\,, \tag{1.51}$$

we end up with the *momentum constraints*

$$D_bK_a{}^b - D_aK = 8\pi S_a. \tag{1.52}$$

As usual we now drop the timelike components,

$$D_jK_i{}^j - D_iK = 8\pi S_i,$$

and then raise indices

$$\begin{aligned}
\gamma^{ki}\left(D_jK_i{}^j - D_iK\right) &= \gamma^{ki}8\pi S_i \\
D_j\left(K^{jk} - \gamma^{jk}K\right) &= 8\pi S^k,
\end{aligned}$$

where we used the compatibility of D with γ_{ab}. This leaves (1.52) in the final form

$$\boxed{D_j\left(K^{ij} - \gamma^{ij}K\right) = 8\pi S^i.} \tag{1.53}$$

Both (1.48) and (1.53) are constraints that need to be satisfied and respected on each time slice Σ. They are restrictions placed on γ_{ab} and K_{ab} so that the spatial slices "fit nicely" when embedded into the ambient spacetime $\mathcal{M}$. We will extensively discuss the *initial data problem* on Chapter 3.

Now, with the evolution of the metric and the constraints taken care of, we move on to find the last key result from this chapter; the evolution equation of K_{ab}. We start by considering its Lie derivative along t^a,

$$\partial_t K_{ab} = \mathcal{L}_{\vec{t}} K_{ab} = \mathcal{L}_{\alpha\vec{n}+\vec{\beta}} K_{ab} = \alpha \mathcal{L}_{\vec{n}} K_{ab} + \mathcal{L}_{\vec{\beta}} K_{ab}.$$

In order to tackle the first term on the RHS, we use Ricci's equation (1.43c)

$$\gamma_a{}^e \gamma_b{}^f n^c n^{d\,(4)} R_{ecfd} = \mathcal{L}_{\vec{n}} K_{ab} + \frac{1}{\alpha} D_a D_b \alpha + K_b{}^c K_{ac},$$

so that

$$\partial_t K_{ab} = \alpha \left(\gamma_a{}^e \gamma_b{}^f n^c n^{d\,(4)} R_{ecfd} - \frac{1}{\alpha} D_a D_b \alpha - K_b{}^c K_{ac} \right) + \mathcal{L}_{\vec{\beta}} K_{ab}. \tag{1.54}$$

Now we should tidy up a bit…First recall that the EFEs ${}^{(4)}G_{ab} = 8\pi T_{ab}$ can be written in the following equivalent way, by contracting with g^{ab}:

$$\begin{aligned} g^{ab\,(4)}G_{ab} = g^{ab\,(4)}R_{ab} - \frac{1}{2}{}^{(4)}R \underbrace{g^{ab} g_{ab}}_{=4} &= 8\pi \underbrace{g^{ab} T_{ab}}_{\equiv T} \\ {}^{(4)}R - 2{}^{(4)}R &= 8\pi T \implies {}^{(4)}R = -8\pi T \\ {}^{(4)}R_{ab} &= 8\pi \left(T_{ab} - \frac{1}{2} T g_{ab} \right), \end{aligned} \tag{1.55}$$

where we defined the *trace of the energy-momentum tensor*

$$T \equiv g^{ab} T_{ab}\,. \tag{1.56}$$

Now note that

$$\begin{aligned} \gamma_a{}^e \gamma_b{}^f n^c n^{d\,(4)} R_{ecfd} &= \gamma_a{}^e \gamma_b{}^f (\gamma^{cd} - g^{cd})\,{}^{(4)}R_{ecfd} \\ &= \gamma_a{}^e \gamma_b{}^f \gamma^{cd\,(4)} R_{ecfd} - \gamma_a{}^e \gamma_b{}^f g^{cd\,(4)} R_{cedf} \\ &= \gamma_a{}^e \gamma_b{}^f \gamma^{cd\,(4)} R_{ecfd} - \gamma_a{}^e \gamma_b{}^{f\,(4)} R_{ef} \\ &= \underbrace{R_{ab} + K K_{ab} - K_{ac} K^c{}_b}_{\text{By (1.44) (contraction of (1.43a))}} \underbrace{- 8\pi \gamma_a{}^e \gamma_b{}^f \left(T_{ef} - \frac{1}{2} T g_{ef} \right)}_{\text{By (1.55)}} \\ &= R_{ab} + K K_{ab} - K_{ac} K^c{}_b - 8\pi \underbrace{\gamma_a{}^e \gamma_b{}^f T_{ef}}_{\equiv S_{ab}\ \text{(spatial stress)}} + 4\pi \underbrace{\gamma_a{}^e \gamma_b{}^f g_{ef}}_{=\gamma_{ab}} \underbrace{T}_{=g^{pr} T_{pr}} \\ &= R_{ab} + K K_{ab} - K_{ac} K^c{}_b - 8\pi S_{ab} + 4\pi \gamma_{ab}\, g^{pr} T_{pr} \\ &= R_{ab} + K K_{ab} - K_{ac} K^c{}_b - 8\pi S_{ab} + 4\pi \gamma_{ab} (\gamma^{pr} - n^p n^r) T_{pr} \\ &= R_{ab} + K K_{ab} - K_{ac} K^c{}_b - 8\pi S_{ab} + 4\pi \gamma_{ab} (\underbrace{\gamma^{pr} T_{pr}}_{=S^a{}_a \equiv S} - \underbrace{n^p n^r T_{pr}}_{=\rho}) \\ &= R_{ab} + K K_{ab} - K_{ac} K^c{}_b - 8\pi S_{ab} + 4\pi \gamma_{ab} (S - \rho). \end{aligned} \tag{1.57}$$

Here we defined the *spatial stress*

$$S_{ab} \equiv \gamma_a{}^c \gamma_b{}^d T_{cd}, \tag{1.58}$$

as well as its trace

$$S \equiv \gamma^{ab} S_{ab} = S^a{}_a. \tag{1.59}$$

Now, inserting the results obtained in (1.57) back into (1.54), we get

$$\begin{aligned}
\partial_t K_{ab} &= \alpha \left(\gamma_a{}^e \gamma_b{}^f n^c n^d\, {}^{(4)}R_{ecfd} - \frac{1}{\alpha} D_a D_b \alpha - K_b{}^c K_{ac}\right) + \mathcal{L}_{\vec{\beta}} K_{ab} \\
&= \alpha (R_{ab} + K K_{ab} - K_{ac} K^c{}_b - 8\pi \left(S_{ab} - \frac{1}{2}\gamma_{ab}(S-\rho)\right) - \frac{1}{\alpha} D_a D_b \alpha \\
&\quad - K_b{}^c K_{ac}) + \mathcal{L}_{\vec{\beta}} K_{ab} \\
&= \alpha (R_{ab} + K K_{ab} - 2K_{ac} K^c{}_b) - 8\pi\alpha \left(S_{ab} - \frac{1}{2}\gamma_{ab}(S-\rho)\right) - D_a D_b \alpha + \mathcal{L}_{\vec{\beta}} K_{ab}.
\end{aligned}$$

Lastly, since the entire content of spatial tensors is available from their spatial components, we can write our results as

$$\boxed{\begin{aligned}
\partial_t K_{ij} = \alpha (R_{ij} + K K_{ij} - 2K_{ik} K^k{}_j) - 8\pi\alpha \left(S_{ij} - \frac{1}{2}\gamma_{ij}(S-\rho)\right) - D_i D_j \alpha \\
+ \beta^k D_k K_{ij} + 2K_{k(i} D_{j)} \beta^k,
\end{aligned}} \tag{1.60}$$

where we used

$$\mathcal{L}_{\vec{\beta}} K_{ij} = \beta^k D_k K_{ij} + K_{kj} D_i \beta^k + K_{ik} D_j \beta^k.$$

Equation (1.60) is the *evolution of the extrinsic curvature*, our last piece of the puzzle.

Now, in theory at least, once we have gravitational field data $\{\gamma_{ij}, K_{ij}\}$ that satisfies the momentum and Hamiltonian constraints on on some initial spatial slice, we may then integrate forward the evolution equations to obtain a spacetime that satisfies the EFEs. In practice, however, numerical stability is highly dependent on gauge choice and initial data prescribed. Moreover, the ADM equations presented above are, in fact, not very stable with respect to constraint violations (this has to do with the degree of *hyperbolicity* of the equations). We will touch on these issues again once we introduce the *BSSN formalism* in the next chapter. For now, let us present a useful contraction of (1.60), namely the evolution of the trace $K \equiv K^a{}_a$:

$$\partial_t K = \alpha \left(4\pi(\rho + S) + K_{ij} K^{ij}\right) - D^2 \alpha + \beta^i \partial_i K, \tag{1.61}$$

where $D^2 = \gamma^{ij} D_i D_j$ is the *spatial Laplace operator*.Let us prove this.

Proof of (1.61). In what follows we will use the Hamiltonian constraint (1.48). Moreover, since we want to expand $\partial_t K = \partial_t(\gamma^{ij} K_{ij}) = \gamma^{ij} \partial_t K_{ij} + K_{ij} \partial_t \gamma^{ij}$, we need the time evolution of the inverse spatial metric. Note that since $\gamma^{ij}\gamma_{jk} = \delta^i{}_k$, we have $\partial_t(\gamma^{ij}\gamma_{jk}) = 0$, which implies

$$\begin{aligned}
\gamma_{jk} \partial_t \gamma^{ij} &= -\gamma^{ij}\, \partial_t \gamma_{jk} \\
\implies \underbrace{\gamma^{lk}\gamma_{jk}}_{=\delta^l{}_j}\, \partial_t \gamma^{ij} &= -\gamma^{lk}\gamma^{ij}\, \partial_t \gamma_{jk} \\
\implies \partial_t \gamma^{il} &= -\gamma^{lk}\gamma^{ij}\, \partial_t \gamma_{jk}.
\end{aligned} \tag{1.62}$$

Now,

$$\begin{aligned}
\partial_t K = \partial_t(\gamma^{ij} K_{ij}) &= \gamma^{ij} \partial_t K_{ij} + K_{ij} \partial_t \gamma^{ij} \\
&= \gamma^{ij} [\alpha (R_{ij} + K K_{ij} - 2K_{ik} K^k{}_j) - 8\pi\alpha \left(S_{ij} - \frac{1}{2}\gamma_{ij}(S-\rho)\right) - D_i D_j \alpha \\
&\quad + \beta^k D_k K_{ij} + K_{kj} D_i \beta^k + K_{ki} D_j \beta^k] + K_{ij}[-\gamma^{jk}\gamma^{im} \partial_t \gamma_{mk}] \\
&= \alpha (\underbrace{R + K^2 - K_{ij}K^{ij}}_{=\,16\pi\rho \text{ by (1.48)}} - K_{ij}K^{ij}) - 8\pi\alpha \left(S - \frac{3}{2}(S-\rho)\right) - D^2\alpha + \beta^i \underbrace{D_i K}_{=\partial_i K} + 2K_{ij} D^i \beta^j \\
&\quad - K^{mk}(-2\alpha K_{mk} + D_m \beta_k + D_k \beta_m)
\end{aligned}$$

$$
\begin{aligned}
&= \alpha(16\pi\rho - K_{ij}K^{ij}) - 8\pi\alpha S + 12\pi\alpha S - 12\pi\alpha\rho - D^2\alpha + \beta^i\partial_i K + 2K_{ij}D^i\beta^j \\
&\quad +2\alpha K_{ij}K^{ij} - \underbrace{\gamma^{nm}\gamma^{lk}K_{nl}\left(D_m\beta_k + D_k\beta_m\right)}_{=2K_{ij}D^i\beta^j} \\
&= \alpha\left(4\pi(\rho + S) + K_{ij}K^{ij}\right) - D^2\alpha + \beta^i\partial_i K. \qquad \spadesuit
\end{aligned}
$$

ADM (à la York) Equations

※ Evolution Equations:

$$
\boxed{
\begin{aligned}
\partial_t\gamma_{ij} &= 2D_{(i}\beta_{j)} - 2\alpha K_{ij} \\
\partial_t K_{ij} &= \alpha(R_{ij} + KK_{ij} - 2K_{ik}K^k{}_j) - 8\pi\alpha\left(S_{ij} - \frac{1}{2}\gamma_{ij}(S-\rho)\right) - D_iD_j\alpha \\
&\quad + \beta^k D_k K_{ij} + 2K_{k(i}D_{j)}\beta^k
\end{aligned}
}
$$

※ Constraint Equations:

$$
\boxed{
\begin{aligned}
R + K^2 - K_{ij}K^{ij} &= 16\pi\rho \\
D_j\left(K^{ij} - \gamma^{ij}K\right) &= 8\pi S^i
\end{aligned}
}
$$

2

The BSSN Formalism

The 3+1 ADM (à la York) decomposition of the EFEs presented in the previous chapter poses a very straightforward, elegant formulation. Unfortunately, however, the EFEs as presented in this form are not quite suitable for numerical implementations. Alas, we need to put in more work before we take a crack at computing anything, since in practice one finds that this form of the 3+1 decomposition results in large instabilities that develop during a computer simulation (this issue is known to be mainly due to the fact that the EFEs in this ADM form are *weakly hyperbolic*; i.e., they are not *well-posed*. [1]) To get around this problem, in an effort to make the EFEs more *strongly hyperbolic* (i.e., more "wave-like"), many modern NR codes utilize the so-called *BSSN* (aka *BSSNOK*) *formalism* which –together with suitable gauge conditions for the lapse and shift– does admit a more robust computational formulation of the EFEs.

In place of the ADM data $\{\gamma_{ij}, K_{ij}\}$, the BSSN formalism splits γ_{ij} into a conformal factor χ and a conformally-related metric $\bar{\gamma}_{ij}$, and it also splits K_{ij} into its trace K and a traceless part A_{ij}. Moreover, three coefficients $\bar{\Gamma}^i$ of the conformal metric are introduced as well. Then, it is these variables that are evolved instead of the original ADM physical quantities…Long story short, the dynamical variables that we consider in the BSSN formalism are

$$\{\chi, \bar{\gamma}_{ij}, \bar{A}_{ij}, K, \bar{\Gamma}^i\}. \tag{2.1}$$

We will present each of these quantities and their evolution equations in this chapter. To that end, let us start by considering a conformal rescaling of the spatial metric of the form

$$\boxed{\begin{aligned} \bar{\gamma}_{ij} &= \chi\gamma_{ij} && (2.2a)\\ \bar{\gamma}^{ij} &= \chi^{-1}\gamma^{ij}, && (2.2b)\end{aligned}}$$

where χ is some positive scaling factor called the *conformal factor*, and the background auxiliary metric $\bar{\gamma}_{ij}$ is known as the *conformally-related metric* (or, simply, the *conformal metric*). Note that the factor for the inverse metric follows naturally from the fact that

$$\bar{\gamma}^{ij}\bar{\gamma}_{jk} = (\chi^{-1}\gamma^{ij})(\chi\gamma_{jk}) = \gamma^{ij}\gamma_{jk} = \delta^i{}_k,$$

so that $\bar{\gamma}^{ij}$ and $\bar{\gamma}_{jk}$ are inverse to each other. It may seem unclear why we scaled the spatial metric in this way, but let it suffice to say that this "trick" will actually yield a convenient and tractable system for the EFEs. Besides the mathematical convenience that such a conformal rescaling brings about, there is also the fact that conformally-related manifolds form an equivalence class, in which objects share certain geometric features. For example, it can be shown that two strongly-causal Lorentzian metrics $g^{(1)}_{ab}$ and $g^{(2)}_{ab}$ for some manifold $\mathcal{M}$ determine the same future and past sets at all points (events) if and only if the two metrics are globally conformal, i.e., if $g^{(1)}_{ab} = \Psi g^{(2)}_{ab}$, for some smooth function $\Psi \in C^\infty(\mathcal{M})$

[1]For more on the concept of hyperbolicity (in the numerical sense), see the detailed analysis on [25].

(see, e.g., [7]). In this case, both spacetimes $(\mathcal{M}, g^{(1)}_{ab})$ and $(\mathcal{M}, g^{(2)}_{ab})$ belong to the same conformal class and share the same causal structure.

A somewhat natural choice for a representative object in a conformal equivalence class of spatial metric tensors would be a metric $\bar{\gamma}_{ij}$ whose determinant is the same as the determinant of a flat metric f_{ij}, in any general chart. Thus, if we adopt a Cartesian coordinate system, we can always enforce that our conformal representative must have unit determinant, i.e., $\bar{\gamma} = 1$. [2] Plugging this back into (2.2), we get

$$1 = \det \bar{\gamma}_{ij} = \det(\chi\gamma_{ij}) = \chi^3 \det \gamma_{ij} = \chi^3\gamma.$$

This would correspond to the choice $\chi = \gamma^{-1/3}$, so that $\gamma_{ij} = \gamma^{1/3}\bar{\gamma}_{ij}$. However note that, since the determinant γ is coordinate-dependent, the conformal factor $\chi = \gamma^{-1/3}$ *is not* a scalar field. In fact, $\bar{\gamma}_{ij}$ is not a tensor field, but rather a *tensor density* of *weight* $-2/3$; we show this now:

Definition 3. *A $\binom{k}{\ell}$ tensor density of weight $\omega \in \mathbb{Q}$ is a quantity $\Xi^{i_1,\dots,i_k}{}_{j_1,\dots,j_\ell}$ that transforms under a change of coordinates as*

$$\Xi^{i'_1,\dots,i'_k}{}_{j'_1,\dots,j'_\ell} = \mathcal{J}^\omega \frac{\partial x^{i'_1}}{\partial x^{i_1}} \cdots \frac{\partial x^{i'_k}}{\partial x^{i_k}} \frac{\partial x^{j_1}}{\partial x^{j'_1}} \cdots \frac{\partial x^{j_\ell}}{\partial x^{j'_\ell}} \, \Xi^{i_1,\dots,i_k}{}_{j_1,\dots,j_\ell} \tag{2.3}$$

where $\mathcal{J}$ is the Jacobian $\mathcal{J} = \det|\partial x^{i'_k}/\partial x^{i_k}|$.

According to this definition then, a tensor field is nothing but a tensor density of weight zero. In our case, we are interested in *spatial* tensor densities; these are regular (zero weight) tensors that multiply a power of the determinant γ. In other words, a *spatial tensor density $\boldsymbol{\tau}$ of weight $\omega \in \mathbb{Q}$* is an object

$$\boldsymbol{\tau} = \gamma^{\omega/2}\boldsymbol{T}, \tag{2.4}$$

where $\boldsymbol{T}$ is a tensor field. Since $\bar{\gamma}_{ij} = \gamma^{-1/3}\gamma_{ij}$, by Eq. (2.4) we have that $\bar{\gamma}_{ij}$ is a tensor density of weight $-2/3$, as we claimed earlier.

To get around this issue of tensor densities, we could introduce a *background flat metric* f_{ij} of Riemannian signature $(+,+,+)$, and set $\chi \equiv (\gamma/f)^{-1/3}$, so that χ becomes a scalar field in this manner, and we could then use non-Cartesian coordinates. However, for our purposes of implementing the standard BSSN formalism, it is convenient to stick to Cartesian coordinates; to see the implementation of this extended BSSN formalism (where non-Cartesian coordinates are used), the reader is referred to [16]. That being said, since we have chosen to deal with tensor densities in our treatment, we must discuss the *Lie derivative of tensor densities*, which is given by

$$\mathcal{L}_{\vec{x}}\boldsymbol{\tau} = [\mathcal{L}_{\vec{x}}\boldsymbol{\tau}]_{\omega=0} + \omega\boldsymbol{\tau}\,\partial_i x^i, \tag{2.5}$$

where the first term is the usual Lie derivative we would compute if $\boldsymbol{\tau}$ had zero weight (i.e., if $\boldsymbol{\tau}$ was a tensor field rather than a tensor density), and ω is the tensor density's weight, as defined above. Likewise, the *covariant derivative of a tensor density* $\boldsymbol{\tau}$ is furnished by [3]

$$\nabla_c\boldsymbol{\tau} = [\nabla_c\boldsymbol{\tau}]_{\omega=0} - \omega\boldsymbol{\tau}\,\Gamma^d_{dc}, \tag{2.6}$$

where, again, the first term is the usual covariant derivative we would compute if τ had zero weight. Using the expression (1.19) we see that, in coordinates, Eq. (2.6) expands as

$$\begin{aligned}(\nabla\boldsymbol{\tau})^{i_1\dots i_a}{}_{j_1\dots j_b c} &= \nabla_c \tau^{i_1\dots i_a}{}_{j_1\dots j_b} \\ &= \partial_c \tau^{i_1\dots i_a}{}_{j_1\dots j_b} + \sum_{d=1}^{a} \tau^{i_1\dots e\dots i_a}{}_{j_1\dots j_b}\Gamma^{i_d}_{ec} - \sum_{d=1}^{b} \tau^{i_1\dots i_a}{}_{j_1\dots e\dots j_b}\Gamma^{e}_{j_d c} - \omega\tau^{i_1\dots i_a}{}_{j_1\dots j_b}\Gamma^d_{dc}.\end{aligned} \tag{2.7}$$

We will frequently encounter Lie- and covariant derivatives of tensor densities in our work.

[2] Here we are using the standard notation $g \equiv \det g_{ab}$, for any metric g_{ab}. (Not to be confused with boldface $\boldsymbol{g}$, which typically denotes the metric tensor g_{ab} itself when using non-index notation. The latter is more common in the mathematics literature.)

[3] Note that the ∇ we are using for this discussion is not necessarily the connection of the 4D spacetime $\mathcal{M}$; this is a rather general discussion, so ∇ can be replaced by whatever affine connection.

Now that we have have presented the conformal factor and some of the subtleties that arise when dealing with tensor densities, it is time to derive our first evolution equation (recall from (2.1) that χ is one of the dynamic variables in the BSSN formalism). We start by recalling the spatial metric evolution (c.f., Eq. (1.37)):

$$\partial_t \gamma_{ij} = -2\alpha K_{ij} + D_i\beta_j + D_j\beta_i.$$

Using this and Jacobi's formula (c.f., Eq. (1.39)), we get

$$\begin{aligned}\partial_t \gamma &= \gamma\gamma^{ij}\partial_t\gamma_{ij} \\ &= \gamma\left(-2\alpha K + 2D_i\beta^i\right).\end{aligned} \tag{2.8}$$

Now, since $D_i\beta^i = \partial_i\beta^i + \Gamma^i_{ij}\beta^j$, with

$$\begin{aligned}\Gamma^i_{ij} &= \frac{1}{2}\gamma^{ik}(\partial_i\gamma_{jk} + \partial_j\gamma_{ik} - \partial_k\gamma_{ij}) \\ &= \frac{1}{2}\gamma^{ik}\partial_j\gamma_{ik}, && \text{(by relabeling)}\end{aligned}$$

we can insert this back into (2.8) to obtain

$$\begin{aligned}\partial_t\gamma &= \gamma\left(-2\alpha K + 2\partial_i\beta^i + \left(\gamma^{ik}\partial_j\gamma_{ik}\right)\beta^j\right) \\ &= \gamma\left(-2\alpha K + 2\partial_i\beta^i + \left(\frac{1}{\gamma}\partial_j\gamma\right)\beta^j\right) \\ &= 2\gamma\left(\partial_i\beta^i - \alpha K\right) + \beta^i\partial_i\gamma.\end{aligned} \tag{2.9}$$

Hence, using $\chi = \gamma^{-1/3}$, we end up with

$$\begin{aligned}\partial_t\chi &= \partial_t\gamma^{-1/3} \\ &= -\frac{1}{3}\gamma^{-4/3}\partial_t\gamma \\ &= -\frac{1}{3}\gamma^{-4/3}\left[2\gamma\left(\partial_i\beta^i - \alpha K\right) + \beta^i\partial_i\gamma\right] && \text{(From Eq. (2.9))} \\ &= -\frac{1}{3}\chi^4\left[2\chi^{-3}\left(\partial_i\beta^i - \alpha K\right) + \beta^i\partial_i\chi^{-3}\right] \\ &= -\frac{2}{3}\chi\left(\partial_i\beta^i - \alpha K\right) - \frac{1}{3}\chi^4\beta^i\cdot(-3)\,\chi^{-4}\partial_i\chi \\ &= \frac{2}{3}\chi(\alpha K - \partial_i\beta^i) + \beta^i\partial_i\chi.\end{aligned}$$

Thus we have derived the *evolution of the conformal factor*:

$$\boxed{\partial_t\chi = \frac{2}{3}\chi(\alpha K - \partial_i\beta^i) + \beta^i\partial_i\chi.} \tag{2.10}$$

Let us now introduce the *traceless part of the extrinsic curvature*, which we denote by A_{ij}, and is given by

$$\boxed{A_{ij} = K_{ij} - \frac{1}{3}\gamma_{ij}K.} \tag{2.11}$$

Note that A_{ij} is indeed traceless: $\gamma^{ij}A_{ij} = \gamma^{ij}\left(K_{ij} - 1/3\gamma_{ij}K\right) = K - 1/3\cdot 3K = K - K = 0$. This way, the extrinsic curvature K_{ij} is naturally split into its trace K and its traceless part A_{ij}:

$$K_{ij} = A_{ij} + \frac{1}{3}\gamma_{ij}K. \tag{2.12}$$

Just as we rescaled the spatial metric in Eq. (2.2), we shall also rescale the traceless curvature A_{ij} as

$$\boxed{\begin{aligned}\bar{A}_{ij} &= \chi A_{ij} && \text{(2.13a)} \\ \bar{A}^{ij} &= \chi^{-1}A^{ij} && \text{(2.13b)}\end{aligned}}$$

which, just as its conformally related A_{ij}, is also traceless:

$$\bar{\gamma}^{ij}\bar{A}_{ij} = \chi\bar{\gamma}^{ij}K_{ij} - \frac{1}{3}\bar{\gamma}^{ij}\bar{\gamma}_{ij}K = \chi\chi^{-1}\gamma^{ij}K_{ij} - \frac{1}{3}\cdot 3K = K - K = 0. \quad \surd$$

This rescaling of the conformal traceless curvature was first considered by Nakamura [20], therefore we will refer to it as the *Nakamura scaling of A_{ij}* (be aware that we shall use a different scaling for A_{ij} when we deal with the initial data problem in the next chapter). This way the conformal version of Eq. (2.11) is

$$\boxed{\bar{A}_{ij} = \chi K_{ij} - \frac{1}{3}\bar{\gamma}_{ij}K.} \tag{2.14}$$

We will refer to $\bar{A}_{ij}$ as the *conformal traceless curvature*. We shall shortly derive its evolution equation (spoiler alert: it is quite messy!), but first let us start with something simpler, such as rewriting the evolution of the trace K in terms of the newly introduced conformal factors. Recall Eq. (1.61),

$$\partial_t K = \alpha\left(4\pi(\rho + S) + K_{ij}K^{ij}\right) - D^2\alpha + \beta^i\partial_i K.$$

Now from (2.14) we write K_{ij} as

$$K_{ij} = \chi^{-1}\left(\bar{A}_{ij} + \frac{1}{3}\bar{\gamma}_{ij}K\right), \tag{2.15}$$

and similarly,

$$\begin{aligned}
K^{ij} &= \gamma^{im}\gamma^{jn}K_{mn} \\
&= \gamma^{im}\gamma^{jn}\chi^{-1}\left(\bar{A}_{mn} + \frac{1}{3}\bar{\gamma}_{mn}K\right) \\
&= \chi^2\bar{\gamma}^{im}\bar{\gamma}^{jn}\chi^{-1}\left(\bar{A}_{mn} + \frac{1}{3}\bar{\gamma}_{mn}K\right) \\
&= \chi\left(\bar{A}^{ij} + \frac{1}{3}\bar{\gamma}^{ij}K\right).
\end{aligned} \tag{2.16}$$

This last equation, by the way, yields the contravariant version of the conformal traceless curvature (2.14):

$$\boxed{\bar{A}^{ij} = \chi^{-1}K^{ij} - \frac{1}{3}\bar{\gamma}^{ij}K.} \tag{2.17}$$

Now, plugging Eqs. (2.15) and (2.16) back into (1.61), we get

$$\begin{aligned}
\partial_t K &= \alpha\left(4\pi(\rho + S) + K_{ij}K^{ij}\right) - D^2\alpha + \beta^i\partial_i K \\
&= \alpha\left[4\pi(\rho + S) + \left(\chi^{-1}\left(\bar{A}_{ij} + \frac{1}{3}\bar{\gamma}_{ij}K\right)\right)\left(\chi\left(\bar{A}^{ij} + \frac{1}{3}\bar{\gamma}^{ij}K\right)\right)\right] - D^2\alpha + \beta^i\partial_i K \\
&= \alpha[4\pi(\rho + S) + \bar{A}_{ij}\bar{A}^{ij} + \underbrace{\frac{1}{3}\bar{A}_{ij}\bar{\gamma}^{ij}K}_{=0\text{ (tracelessness of }\bar{A}_{ij})} + \underbrace{\frac{1}{3}\bar{A}^{ij}\bar{\gamma}_{ij}K}_{=0\text{ (tracelessness of }\bar{A}_{ij})} + \frac{1}{9}\underbrace{\bar{\gamma}_{ij}\bar{\gamma}^{ij}}_{=3}K^2] - D^2\alpha + \beta^i\partial_i K \\
&= \alpha\left(4\pi(\rho + S) + \bar{A}_{ij}\bar{A}^{ij} + \frac{1}{3}K^2\right) - D^2\alpha + \beta^i\partial_i K.
\end{aligned}$$

And thus we have the *evolution of the trace of the extrinsic curvature*:

$$\boxed{\partial_t K = \alpha\left(\bar{A}_{ij}\bar{A}^{ij} + \frac{1}{3}K^2\right) + 4\pi\alpha(\rho + S) - D^2\alpha + \beta^i\partial_i K.} \tag{2.18}$$

Note, however, that in this equation we are using covariant derivatives D of the lapse with respect to the physical metric γ_{ij}, even though we would like to write everything in this expression in terms of the conformal metric $\bar{\gamma}_{ij}$. We will fix this issue later once we introduce the conformal connection $\bar{D}$ of $\bar{\gamma}_{ij}$ (c.f., Eq. (2.32)).

Now, before tackling the evolution of $\bar{A}_{ij}$, we need to clarify a few things. First note that

$$K^k{}_j = \gamma^{ki}K_{ij} = \chi\bar{\gamma}^{ki}K_{ij} = \chi\bar{\gamma}^{ki}\chi^{-1}\left(\bar{A}_{ij} + \frac{1}{3}\bar{\gamma}_{ij}K\right) = \bar{A}^k{}_j + \delta^k{}_j K.$$

We will use this in the calculations that follow, just as we will also use the notation $[\cdots]^{\mathrm{TF}}$ to denote the trace-free part of whatever object lies inside the brackets (e.g., $[K_{ij}]^{\mathrm{TF}} = A_{ij}$). In general, for a tensor $\boldsymbol{T}$ in a D-dimensional metric $\boldsymbol{g}$, we have $[\boldsymbol{T}]^{\mathrm{TF}} = \boldsymbol{T} - \boldsymbol{g}/D\,\mathrm{Tr}(\boldsymbol{T})$ (we have already used this when we defined A_{ij} in (2.11)). Naturally, it follows that if $\boldsymbol{T}$ is already trace-free, then $[\boldsymbol{T}]^{\mathrm{TF}} = \boldsymbol{T}$. Furthermore, we will also use the fact that the metric tensor does not contain any trace-free part (for instance, for $\bar{\gamma}_{ij}$, we have $[\bar{\gamma}_{ij}]^{\mathrm{TF}} = \bar{\gamma}_{ij} - \bar{\gamma}_{ij}/3\,\mathrm{Tr}(\bar{\gamma}_{ij}) = \bar{\gamma}_{ij} - \bar{\gamma}_{ij}/3\cdot 3 = 0$). Lastly, we also note that since $\bar{A}_{ij}$ and χ^{-1} are tensor densities of weights $-2/3$ and $2/3$, respectively (c.f., Eq. (2.4)), their Lie derivatives are given by

$$\mathcal{L}_{\vec{\beta}}\bar{A}_{ij} = \beta^k\partial_k\bar{A}_{ij} + \bar{A}_{ik}\partial_j\beta^k + \bar{A}_{kj}\partial_i\beta^k - \frac{2}{3}\bar{A}_{ij}\partial_k\beta^k, \tag{2.19}$$

$$\begin{aligned}\mathcal{L}_{\vec{\beta}}\chi^{-1} &= \beta^k\partial_k\chi^{-1} + \frac{2}{3}\chi^{-1}\partial_k\beta^k \\ &= -\chi^{-2}\beta^k\partial_k\chi + \frac{2}{3}\chi^{-1}\partial_k\beta^k.\end{aligned} \tag{2.20}$$

Now we are (at last!) ready to calculate the evolution of $\bar{A}_{ij}$:

$$\begin{aligned}
\partial_t\bar{A}_{ij} &= \partial_t(\chi A_{ij}) = \chi\partial_t A_{ij} + A_{ij}\partial_t\chi \\
&= \chi[\partial_t K_{ij}]^{\mathrm{TF}} + A_{ij}\partial_t\chi \\
&= \chi\left[\alpha(R_{ij} + KK_{ij} - 2K_{ik}K^k{}_j) - 8\pi\alpha(S_{ij} - \frac{1}{2}\underbrace{\gamma_{ij}}_{\text{no TF}}(S-\rho)) - D_iD_j\alpha + \mathcal{L}_{\vec{\beta}}K_{ij}\right]^{\mathrm{TF}} \\
&\quad + \chi^{-1}\bar{A}_{ij}\left[\frac{2}{3}\chi(\alpha K - \partial_i\beta^i) + \beta^i\partial_i\chi\right] \\
&= [\alpha\chi R_{ij} + \alpha\chi\chi^{-1}K\left(\bar{A}_{ij} + \frac{1}{3}\bar{\gamma}_{ij}K\right) - 2\alpha\chi\chi^{-1}\left(\bar{A}_{ik} + \frac{1}{3}\bar{\gamma}_{ik}K\right)\left(\bar{A}^k{}_j + \delta^k{}_jK\right)\dots \\
&\quad \dots - 8\pi\alpha\chi S_{ij} - \chi D_iD_j\alpha]^{\mathrm{TF}} + \chi\underbrace{[\mathcal{L}_{\vec{\beta}}K_{ij}]^{\mathrm{TF}}}_{=\mathcal{L}_{\vec{\beta}}A_{ij}} + \frac{2}{3}\bar{A}_{ij}\alpha K - \frac{2}{3}\bar{A}_{ij}\partial_k\beta^k + \bar{A}_{ij}\chi^{-1}\beta^k\partial_k\chi \\
&= [\alpha\chi R_{ij} + \alpha K\bar{A}_{ij} + \frac{1}{3}\alpha\underbrace{\bar{\gamma}_{ij}}_{\text{no TF}}K^2 - 2\alpha\bar{A}_{ik}\bar{A}^k{}_j - 2\alpha K\bar{A}_{ij} - \frac{2}{3}\alpha K\bar{A}_{ij} - \frac{2}{3}\alpha\underbrace{\bar{\gamma}_{ij}}_{\text{no TF}}K^2\dots \\
&\quad \dots - 8\pi\alpha\chi S_{ij} - \chi D_iD_j\alpha]^{\mathrm{TF}} + \chi\underbrace{\mathcal{L}_{\vec{\beta}}A_{ij}}_{=\mathcal{L}_{\vec{\beta}}(\chi^{-1}\bar{A}_{ij})} + \frac{2}{3}\bar{A}_{ij}\alpha K - \frac{2}{3}\bar{A}_{ij}\partial_k\beta^k + \bar{A}_{ij}\chi^{-1}\beta^k\partial_k\chi \\
&= \left[\alpha\chi R_{ij} + \alpha K\bar{A}_{ij} - 2\alpha\bar{A}_{ik}\bar{A}^k{}_j - 2\alpha K\bar{A}_{ij} - \frac{2}{3}\alpha K\bar{A}_{ij} - 8\pi\alpha\chi S_{ij} - \chi D_iD_j\alpha\right]^{\mathrm{TF}} \\
&\quad + \chi\mathcal{L}_{\vec{\beta}}(\chi^{-1}\bar{A}_{ij}) + \frac{2}{3}\bar{A}_{ij}\alpha K - \frac{2}{3}\bar{A}_{ij}\partial_k\beta^k + \bar{A}_{ij}\chi^{-1}\beta^k\partial_k\chi \\
&= \left[\alpha\chi R_{ij} - 8\pi\alpha\chi S_{ij} - \chi D_iD_j\alpha\right]^{\mathrm{TF}} - 2\alpha\bar{A}_{ik}\bar{A}^k{}_j - \alpha K\bar{A}_{ij} - \frac{2}{3}\alpha K\bar{A}_{ij} + \frac{2}{3}\alpha K\bar{A}_{ij} \\
&\quad + \chi\chi^{-1}\mathcal{L}_{\vec{\beta}}\bar{A}_{ij} + \bar{A}_{ij}\chi\mathcal{L}_{\vec{\beta}}\chi^{-1} - \frac{2}{3}\bar{A}_{ij}\partial_k\beta^k + \bar{A}_{ij}\chi^{-1}\beta^k\partial_k\chi \\
&= \left[\chi(\alpha R_{ij} - 8\pi\alpha S_{ij} - D_iD_j\alpha)\right]^{\mathrm{TF}} - \alpha(2\bar{A}_{ik}\bar{A}^k{}_j + \bar{A}_{ij}K) + \mathcal{L}_{\vec{\beta}}\bar{A}_{ij} \\
&\quad + \bar{A}_{ij}\chi\left(-\chi^{-2}\beta^k\partial_k\chi + \frac{2}{3}\chi^{-1}\partial_k\beta^k\right) - \frac{2}{3}\bar{A}_{ij}\partial_k\beta^k + \bar{A}_{ij}\chi^{-1}\beta^k\partial_k\chi \\
&= \left[\chi(\alpha R_{ij} - 8\pi\alpha S_{ij} - D_iD_j\alpha)\right]^{\mathrm{TF}} - \alpha(2\bar{A}_{ik}\bar{A}^k{}_j + \bar{A}_{ij}K) + \mathcal{L}_{\vec{\beta}}\bar{A}_{ij}.
\end{aligned}$$

After all this mess(!) and evaluating $\mathcal{L}_{\vec{\beta}}\bar{A}_{ij}$ by Eq. (2.19), we arrive at our sought-after *evolution of the conformal traceless curvature*.

$$\boxed{\begin{aligned}\partial_t\bar{A}_{ij} = &\left[\chi(\alpha R_{ij} - 8\pi\alpha S_{ij} - D_iD_j\alpha)\right]^{\mathrm{TF}} - \alpha(2\bar{A}_{ik}\bar{A}^k{}_j + \bar{A}_{ij}K)\\ &+ \beta^k\partial_k\bar{A}_{ij} + \bar{A}_{ik}\partial_j\beta^k + \bar{A}_{kj}\partial_i\beta^k - \frac{2}{3}\bar{A}_{ij}\partial_k\beta^k.\end{aligned}} \tag{2.21}$$

Without the $[\cdots]^{\mathrm{TF}}$ notation, we can write this as

$$\begin{aligned}\partial_t\bar{A}_{ij} = &\chi\left[\left(\alpha\left(R_{ij} - \frac{1}{3}\gamma_{ij}R\right) - 8\pi\alpha\left(S_{ij} - \frac{1}{3}\gamma_{ij}S\right) - (D_iD_j\alpha - \frac{1}{3}\gamma_{ij}D^2\alpha)\right]\\ &- \alpha(2\bar{A}_{ik}\bar{A}^k{}_j + \bar{A}_{ij}K) + \beta^k\partial_k\bar{A}_{ij} + \bar{A}_{ik}\partial_j\beta^k + \bar{A}_{kj}\partial_i\beta^k - \frac{2}{3}\bar{A}_{ij}\partial_k\beta^k.\end{aligned}$$

Once again, just as it was the case for the evolution equation of K (c.f., (2.18)), we have covariant derivatives D of the lapse with respect to the physical metric γ_{ij} (moreover, this time we also have the 3D Ricci tensor R_{ij} of γ_{ij} appearing in the expression). We will correct these problems soon by introducing the conformal connection $\bar{D}$ of $\bar{\gamma}_{ij}$ and rewriting everything in terms of the conformal metric.

The conformal traceless curvature $\bar{A}_{ij}$ shows up in the evolution of the conformal metric $\bar{\gamma}_{ij}$, which we shall now derive. To do so, we use Eq. (1.3) and the fact that $\mathcal{L}_{\vec{t}} = \partial_t$ in our adapted coordinates to write

$$\partial_t\bar{\gamma}_{ij} = \mathcal{L}_{\vec{t}}\bar{\gamma}_{ij} = \alpha\mathcal{L}_{\vec{n}}\bar{\gamma}_{ij} + \mathcal{L}_{\vec{\beta}}\bar{\gamma}_{ij}. \tag{2.22}$$

To expand the second term on the RHS, we note that it is a Lie derivative of a tensor density of weight $-2/3$; thus we use Eq. (2.5) to get

$$\mathcal{L}_{\vec{\beta}}\bar{\gamma}_{ij} = \beta^k\partial_k\bar{\gamma}_{ij} + \bar{\gamma}_{ik}\partial_j\beta^k + \bar{\gamma}_{kj}\partial_i\beta^k - \frac{2}{3}\bar{\gamma}_{ij}\partial_k\beta^k. \tag{2.23}$$

Better yet, we can write this Lie derivative in terms of the conformal connection $\bar{D}$ (defined below; c.f., Eq. (2.28)). In this calculation we will need to expand the covariant derivative of $\bar{\gamma}_{ij}$ using the formula for the covariant derivative of a tensor density (c.f., Eq. (2.7)):

$$\bar{D}_k\bar{\gamma}_{ij} = \partial_k\bar{\gamma}_{ij} - \bar{\Gamma}^\ell_{ik}\bar{\gamma}_{\ell j} - \bar{\Gamma}^\ell_{jk}\bar{\gamma}_{i\ell} + \frac{2}{3}\bar{\gamma}_{ij}\bar{\Gamma}^\ell_{\ell k}.$$

Let us now expand (2.23),

$$\begin{aligned}\mathcal{L}_{\vec{\beta}}\bar{\gamma}_{ij} &= \beta^k\partial_k\bar{\gamma}_{ij} + \bar{\gamma}_{ik}\partial_j\beta^k + \bar{\gamma}_{kj}\partial_i\beta^k - \frac{2}{3}\bar{\gamma}_{ij}\partial_k\beta^k\\ &= \beta^k\underbrace{\bar{D}_k\bar{\gamma}_{ij}}_{=0} + \beta^k\bar{\Gamma}^\ell_{ik}\bar{\gamma}_{\ell j} + \beta^k\bar{\Gamma}^\ell_{jk}\bar{\gamma}_{i\ell} - \frac{2}{3}\bar{\gamma}_{ij}\bar{\Gamma}^\ell_{\ell k}\beta^k + \underbrace{\bar{\gamma}_{ik}\bar{D}_j\beta^k}_{=\bar{D}_j\beta_i} - \bar{\gamma}_{ik}\bar{\Gamma}^k_{\ell j}\beta^\ell\\ &\quad + \underbrace{\bar{\gamma}_{kj}\bar{D}_i\beta^k}_{=\bar{D}_i\beta_j} - \bar{\gamma}_{kj}\bar{\Gamma}^k_{\ell i}\beta^\ell - \frac{2}{3}\bar{\gamma}_{ij}\bar{D}_k\beta^k + \frac{2}{3}\bar{\gamma}_{ij}\bar{\Gamma}^k_{\ell k}\beta^\ell\\ &= \underbrace{\beta^k\bar{\Gamma}^\ell_{ik}\bar{\gamma}_{\ell j} + \beta^k\bar{\Gamma}^\ell_{jk}\bar{\gamma}_{i\ell} - \frac{2}{3}\bar{\gamma}_{ij}\bar{\Gamma}^\ell_{\ell k}\beta^k - \bar{\gamma}_{ik}\bar{\Gamma}^k_{\ell j}\beta^\ell - \bar{\gamma}_{kj}\bar{\Gamma}^k_{\ell i}\beta^\ell + \frac{2}{3}\bar{\gamma}_{ij}\bar{\Gamma}^k_{\ell k}\beta^\ell}_{=\,0\text{ by relabeling}} + 2\bar{D}_{(i}\beta_{j)} - \frac{2}{3}\bar{\gamma}_{ij}\bar{D}_k\beta^k\\ &= 2\bar{D}_{(i}\beta_{j)} - \frac{2}{3}\bar{\gamma}_{ij}\bar{D}_k\beta^k.\end{aligned} \tag{2.24}$$

And now we tackle the first term on the RHS of (2.22):

$$\begin{aligned}
\alpha \mathcal{L}_{\vec{n}} \bar{\gamma}_{ij} &= \alpha \mathcal{L}_{\vec{n}} (\chi \gamma_{ij}) \\
&= \alpha (\chi \underbrace{\mathcal{L}_{\vec{n}} \gamma_{ij}}_{=-2K_{ij}} + \gamma_{ij} \mathcal{L}_{\vec{n}} \chi) \\
&= -2\alpha\chi K_{ij} + \alpha \gamma_{ij} \frac{1}{\alpha} (\underbrace{\mathcal{L}_{\vec{t}}}_{\partial_t} \chi - \mathcal{L}_{\vec{\beta}} \chi) \\
&= -2\alpha\chi \left(\chi^{-1} \left(\bar{A}_{ij} + \frac{1}{3} \bar{\gamma}_{ij} K \right) \right) + \gamma_{ij} \left(\frac{2}{3} \chi (\alpha K - \partial_k \beta^k) + \beta^k \partial_k \chi - \left(\beta^k \partial_k \chi - \frac{2}{3} \chi \partial_k \beta^k \right) \right) \\
&= -2\alpha \bar{A}_{ij} - \frac{2}{3} \alpha \chi \gamma_{ij} K + \frac{2}{3} \alpha \chi \gamma_{ij} K - \frac{2}{3} \chi \gamma_{ij} \partial_k \beta^k + \frac{2}{3} \chi \gamma_{ij} \partial_k \beta^k + \gamma_{ij} \beta^k \partial_k \chi - \gamma_{ij} \beta^k \partial_k \chi \\
&= -2\alpha \bar{A}_{ij}.
\end{aligned} \tag{2.25}$$

Hence, combining Eqs. (2.25) and (2.24), equation (2.22) yields the *evolution of the conformal metric*:

$$\boxed{\partial_t \bar{\gamma}_{ij} = -2\alpha \bar{A}_{ij} + 2\bar{D}_{(i}\beta_{j)} - \frac{2}{3} \bar{\gamma}_{ij} \bar{D}_k \beta^k.} \tag{2.26}$$

We are now down to the last item from (2.1), namely, the coefficients $\bar{\Gamma}^i \equiv \bar{\gamma}^{jk} \bar{\Gamma}^i_{jk}$ of the conformal metric $\bar{\gamma}_{ij}$, where

$$\bar{\Gamma}^i_{jk} = \frac{1}{2} \bar{\gamma}^{i\ell} \left(\partial_j \bar{\gamma}_{\ell k} + \partial_k \bar{\gamma}_{\ell j} - \partial_\ell \bar{\gamma}_{jk} \right). \tag{2.27}$$

These symbols are the connection coefficients of the *conformal connection* $\bar{D}$ of $\bar{\gamma}_{ij}$, from which (analogous to Eq. (1.19)) we define the *conformal spatial derivative* $\bar{D}_a$ of some $\binom{a}{b}$ tensor field $\boldsymbol{T}$ in a coordinate chart as [4]

$$\begin{aligned}
(\bar{D}\boldsymbol{T})^{i_1 \dots i_a}{}_{j_1 \dots j_b c} &= \bar{D}_c T^{i_1 \dots i_a}{}_{j_1 \dots j_b} \\
&= \partial_c T^{i_1 \dots i_a}{}_{j_1 \dots j_b} + \sum_{d=1}^{a} T^{i_1 \dots e \dots i_a}{}_{j_1 \dots j_b} \bar{\Gamma}^{i_d}_{ec} - \sum_{d=1}^{b} T^{i_1 \dots i_a}{}_{j_1 \dots e \dots j_b} \bar{\Gamma}^{e}_{j_d c}.
\end{aligned} \tag{2.28}$$

We first note that in Cartesian coordinates, where $\bar{\gamma} = 1$, we have

$$\begin{aligned}
\bar{\Gamma}^i &= \bar{\gamma}^{jk} \bar{\Gamma}^i_{jk} \\
&= \bar{\gamma}^{jk} \left[\frac{1}{2} \bar{\gamma}^{i\ell} \left(\partial_j \bar{\gamma}_{\ell k} + \partial_k \bar{\gamma}_{\ell j} - \partial_\ell \bar{\gamma}_{jk} \right) \right] \\
&= -\frac{1}{2} \underbrace{\bar{\gamma}^{jk} \bar{\gamma}_{\ell k}}_{= \delta^j{}_\ell} \partial_j \bar{\gamma}^{i\ell} - \frac{1}{2} \underbrace{\bar{\gamma}^{jk} \bar{\gamma}_{\ell j}}_{= \delta^k{}_\ell} \partial_k \bar{\gamma}^{i\ell} - \frac{1}{2} \bar{\gamma}^{i\ell} \underbrace{\bar{\gamma}^{jk} \partial_\ell \bar{\gamma}_{jk}}_{= 0 \text{ by (2.30)}} \\
&= -\frac{1}{2} \partial_\ell \bar{\gamma}^{i\ell} - \frac{1}{2} \partial_\ell \bar{\gamma}^{i\ell} \\
&= -\partial_j \bar{\gamma}^{ij},
\end{aligned} \tag{2.29}$$

where we used

$$\partial_j (\bar{\gamma}^{i\ell} \bar{\gamma}_{\ell k}) = \partial_j \delta^i{}_k = 0 \implies \bar{\gamma}^{i\ell} \partial_j \bar{\gamma}_{\ell k} = -\bar{\gamma}_{\ell k} \partial_j \bar{\gamma}^{i\ell},$$

as well as Jacobi's formula (c.f. Eq. (1.39)):

$$\bar{\gamma}^{jk} \partial_\ell \bar{\gamma}_{jk} = \frac{1}{\bar{\gamma}} \partial_\ell \bar{\gamma} \overset{\text{since } \bar{\gamma} = 1}{=\!=\!=\!=\!=} 0. \tag{2.30}$$

[4]Note, however, that due to the tensor density nature of $\bar{\gamma}_{ij}$, the connection $\bar{D}$ is not unique (i.e., it is not a Levi-Civita connection). Nevertheless, it *is* compatible with the conformal metric; i.e., $\bar{D}_k \bar{\gamma}_{ij} = 0$.

The conversion from the Christoffel symbols Γ^i_{jk} of the spatial metric γ_{ij} to the conformal symbols $\bar{\Gamma}^i_{jk}$ of the conformal metric $\bar{\gamma}_{ij}$ is given as follows:

$$\begin{aligned}
\Gamma^i_{jk} &= \frac{1}{2}\gamma^{i\ell}\left(\partial_j\gamma_{\ell k} + \partial_k\gamma_{\ell j} - \partial_\ell\gamma_{jk}\right) \\
&= \frac{1}{2}\chi\bar{\gamma}^{i\ell}\left(\partial_j(\chi^{-1}\bar{\gamma}_{\ell k}) + \partial_k(\chi^{-1}\bar{\gamma}_{\ell j}) - \partial_\ell(\chi^{-1}\bar{\gamma}_{jk})\right) \\
&= \frac{1}{2}\chi\bar{\gamma}^{i\ell}\left(\chi^{-1}\,\partial_j\bar{\gamma}_{\ell k} + \bar{\gamma}_{\ell k}\,\partial_j\chi^{-1} + \chi^{-1}\,\partial_k\bar{\gamma}_{\ell j} + \bar{\gamma}_{\ell j}\,\partial_k\chi^{-1} - \chi^{-1}\,\partial_\ell\bar{\gamma}_{jk} - \bar{\gamma}_{jk}\,\partial_\ell\chi^{-1}\right) \\
&= \underbrace{\frac{1}{2}\bar{\gamma}^{i\ell}\left(\partial_j\bar{\gamma}_{\ell k} + \partial_k\bar{\gamma}_{\ell j} - \partial_\ell\bar{\gamma}_{jk}\right)}_{=\bar{\Gamma}^i_{jk}} + \frac{1}{2}\chi\bar{\gamma}^{i\ell}\left(-\chi^{-2}\bar{\gamma}_{\ell k}\,\partial_j\chi - \chi^{-2}\bar{\gamma}_{\ell j}\,\partial_k\chi + \chi^{-2}\bar{\gamma}_{jk}\,\partial_\ell\chi\right) \\
&= \bar{\Gamma}^i_{jk} - \frac{1}{2}\chi^{-1}\left(\delta^i{}_k\,\partial_j\chi + \delta^i{}_j\,\partial_k\chi - \bar{\gamma}_{jk}\bar{\gamma}^{i\ell}\,\partial_\ell\chi\right).
\end{aligned} \tag{2.31}$$

Now it is time to rectify the issues we alluded to earlier regarding the spatial covariant derivative of the lapse and the spatial Ricci tensor showing up in equations where every other term is written in terms of the conformal factors (see comments below Eqs. (2.18) and (2.21)):

※ **[Spatial Derivative]** Using (2.31), we expand the term $D_iD_j\alpha$ that appears both in the evolution of K (2.18) and in the evolution of $\bar{A}_{ij}$ (2.21):

$$\begin{aligned}
D_iD_j\alpha = D_i\partial_j\alpha &= \partial_i\partial_j\alpha - \Gamma^k_{ij}\partial_k\alpha \\
&= \partial_i\partial_j\alpha - \left[\bar{\Gamma}^k_{ij} - \frac{1}{2}\chi^{-1}\left(\delta^k{}_i\,\partial_j\chi + \delta^k{}_j\,\partial_i\chi - \bar{\gamma}_{ij}\bar{\gamma}^{k\ell}\,\partial_\ell\chi\right)\right]\partial_k\alpha \\
&= \partial_i\partial_j\alpha - \bar{\Gamma}^k_{ij}\,\partial_k\alpha + \frac{1}{2\chi}\left(2\partial_{(i}\chi\partial_{j)}\alpha - \bar{\gamma}_{ij}\bar{\gamma}^{k\ell}\,\partial_\ell\chi\,\partial_k\alpha\right).
\end{aligned}$$

Then, using the fact that both χ and α are treated as scalars when taking covariant derivatives, we get the final expression

$$\boxed{D_iD_j\alpha = \bar{D}_i\bar{D}_j\alpha + \frac{1}{2\chi}\left(2\bar{D}_{(i}\chi\bar{D}_{j)}\alpha - \bar{\gamma}_{ij}\,\bar{D}_k\chi\,\bar{D}^k\alpha\right).} \tag{2.32}$$

※ **[Spatial Ricci Tensor]** The 3D (spatial) Ricci tensor can be split into the conformal Ricci tensor

$$\bar{R}_{ij} = \partial_k\bar{\Gamma}^k_{ij} - \partial_j\bar{\Gamma}^k_{ik} + \bar{\Gamma}^k_{\ell k}\,\bar{\Gamma}^\ell_{ij} - \bar{\Gamma}^k_{\ell j}\,\bar{\Gamma}^\ell_{ik} \tag{2.33}$$

and some extra terms that arise as a result of the rescaling of the metric. The whole derivation of this split of the Ricci tensor requires quite a bit of work, however, so instead of straying too far off here on a tangent, the reader may refer to Appendix B, where everything is derived in great detail. Here we will simply quote the result obtained in the appendix: R_{ij} can be split as

$$R_{ij} = \bar{R}_{ij} + R^\chi_{ij},$$

where $\bar{R}_{ij}$ is given by Eq. (2.33), and R^χ_{ij} is given by

$$\begin{aligned}
R^\chi_{ij} &= \frac{1}{2}\left(\bar{D}_i\bar{D}_j(\log\chi) + \bar{\gamma}_{ij}\,\bar{D}_k\bar{D}^k(\log\chi)\right) \\
&\quad + \frac{1}{4}\left(\bar{D}_i(\log\chi)\bar{D}_j(\log\chi) - \bar{\gamma}_{ij}\,\bar{D}_k(\log\chi)\bar{D}^k(\log\chi)\right).
\end{aligned}$$

Moreover, making use of the newly introduced coefficients $\bar{\Gamma}^i$, Eq. (2.33) may be rewritten as

$$\bar{R}_{ij} = -\frac{1}{2}\bar{\gamma}^{k\ell}\partial_k\partial_\ell\bar{\gamma}_{ij} + \bar{\gamma}_{k(i}\partial_{j)}\,\bar{\Gamma}^k + \bar{\Gamma}^k\,\bar{\Gamma}_{(ij)k} + \bar{\gamma}^{k\ell}\left(2\,\bar{\Gamma}^m_{k(i}\bar{\Gamma}_{j)m\ell} + \bar{\Gamma}^m_{ik}\,\bar{\Gamma}_{j\ell m}\right).$$

The reason why we want to write $\bar{R}_{ij}$ in this form is because, with the exception of the Laplacian term $\bar{\gamma}^{k\ell}\partial_k\partial_\ell\bar{\gamma}_{ij}$, every other second derivative of the metric $\bar{\gamma}_{ij}$ is being absorbed into first derivatives of $\bar{\Gamma}^i$. This in turns makes the BSSN equations more "wave-like" (i.e., *hyperbolic*; see, e.g., [25]). We sum up our discussion on this segment here:

$$\boxed{\begin{aligned} R_{ij} &= \bar{R}_{ij} + R^\chi_{ij} && \text{(2.34a)}\\ \bar{R}_{ij} &= -\frac{1}{2}\bar{\gamma}^{k\ell}\partial_k\partial_\ell\bar{\gamma}_{ij} + \bar{\gamma}_{k(i}\partial_{j)}\bar{\Gamma}^k + \bar{\Gamma}^k\,\bar{\Gamma}_{(ij)k} + \bar{\gamma}^{k\ell}\left(2\,\bar{\Gamma}^m_{k(i}\bar{\Gamma}_{j)m\ell} + \bar{\Gamma}^m_{ik}\,\bar{\Gamma}_{j\ell m}\right) && \text{(2.34b)}\\ R^\chi_{ij} &= \frac{1}{2}\left(\bar{D}_i\bar{D}_j(\log\chi) + \bar{\gamma}_{ij}\,\bar{D}_k\bar{D}^k(\log\chi)\right) && \text{(2.34c)}\\ &\quad + \frac{1}{4}\left(\bar{D}_i(\log\chi)\bar{D}_j(\log\chi) - \bar{\gamma}_{ij}\,\bar{D}_k(\log\chi)\bar{D}^k(\log\chi)\right). \end{aligned}}$$

The expression for the lapse derivative (2.32) is to be inserted into both (2.18) and (2.21), in addition to the split of the Ricci tensor (2.34) being inserted into (2.21). This fixes the issues we brought up earlier.

Now, by writing $\bar{R}_{ij}$ in the form presented on Eq. (2.34b), we are making the $\bar{\Gamma}^i$ independent variables; therefore an evolution equation for these coefficients must be derived as well. To that end, using Eq. (2.29), we start by writing

$$\partial_t\bar{\Gamma}^i = \partial_t(-\partial_j\bar{\gamma}^{ij}) = -\partial_j\partial_t\bar{\gamma}^{ij},$$

where on the last line we used the fact that ordinary partial derivatives commute. Naturally, we now need an evolution equation for the inverse conformal metric; to that end we proceed as we did for Eq. (1.62): note that since $\bar{\gamma}^{ij}\bar{\gamma}_{jk} = \delta^i{}_k$, we have $\partial_t(\bar{\gamma}^{ij}\bar{\gamma}_{jk}) = 0$, which implies

$$\begin{aligned} \bar{\gamma}_{jk}\partial_t\bar{\gamma}^{ij} &= -\bar{\gamma}^{ij}\,\partial_t\bar{\gamma}_{jk}\\ \Longrightarrow\ \underbrace{\bar{\gamma}^{lk}\bar{\gamma}_{jk}}_{=\delta^l{}_j}\,\partial_t\bar{\gamma}^{ij} &= -\bar{\gamma}^{lk}\bar{\gamma}^{ij}\,\partial_t\bar{\gamma}_{jk}\\ \Longrightarrow\ \partial_t\bar{\gamma}^{il} &= -\bar{\gamma}^{lk}\bar{\gamma}^{ij}\,\partial_t\bar{\gamma}_{jk}. \end{aligned}$$

Hence we have

$$\partial_t\bar{\Gamma}^i = -\partial_j\partial_t\bar{\gamma}^{ij} = -\partial_j\left(-\bar{\gamma}^{ik}\bar{\gamma}^{j\ell}\,\partial_t\bar{\gamma}_{k\ell}\right). \tag{2.35}$$

Now recall the evolution of conformal metric,

$$\partial_t\bar{\gamma}_{k\ell} = -2\alpha\bar{A}_{k\ell} + \mathcal{L}_{\vec{\beta}}\bar{\gamma}_{k\ell} = -2\alpha\bar{A}_{k\ell} + \beta^m\partial_m\bar{\gamma}_{k\ell} + \bar{\gamma}_{km}\partial_\ell\beta^m + \bar{\gamma}_{\ell m}\partial_k\beta^m - \frac{2}{3}\bar{\gamma}_{k\ell}\partial_m\beta^m,$$

and note the following fact:

$$\begin{aligned} \partial_m\bar{\gamma}^{ij} &= \partial_m\left(\bar{\gamma}^{ik}\bar{\gamma}^{j\ell}\bar{\gamma}_{k\ell}\right)\\ &= \bar{\gamma}^{ik}\bar{\gamma}^{j\ell}\,\partial_m\bar{\gamma}_{k\ell} + \underbrace{\bar{\gamma}^{ik}\bar{\gamma}_{k\ell}}_{=\delta^i{}_\ell}\,\partial_m\bar{\gamma}^{j\ell} + \underbrace{\bar{\gamma}^{j\ell}\bar{\gamma}_{k\ell}}_{=\delta^j{}_k}\,\partial_m\bar{\gamma}^{ik}\\ &= \bar{\gamma}^{ik}\bar{\gamma}^{j\ell}\,\partial_m\bar{\gamma}_{k\ell} + 2\partial_m\bar{\gamma}^{ij}\\ \Longrightarrow\ \bar{\gamma}^{ik}\bar{\gamma}^{j\ell}\,\partial_m\bar{\gamma}_{k\ell} &= -\partial_m\bar{\gamma}^{ij}. \end{aligned}$$

Now expand Eq. (2.35):

$$\begin{aligned} \partial_t\bar{\Gamma}^i &= -\partial_j\left(-\bar{\gamma}^{ik}\bar{\gamma}^{j\ell}\,\partial_t\bar{\gamma}_{k\ell}\right)\\ &= \partial_j\left[\bar{\gamma}^{ik}\bar{\gamma}^{j\ell}\left(-2\alpha\bar{A}_{k\ell} + \beta^m\partial_m\bar{\gamma}_{k\ell} + \bar{\gamma}_{km}\partial_\ell\beta^m + \bar{\gamma}_{\ell m}\partial_k\beta^m - \frac{2}{3}\bar{\gamma}_{k\ell}\partial_m\beta^m\right)\right] \end{aligned}$$

$$
\begin{aligned}
&= \partial_j \left(-2\alpha \bar{A}^{ij} - \beta^m \partial_m \bar{\gamma}^{ij} + \bar{\gamma}^{j\ell}\partial_\ell \beta^i + \bar{\gamma}^{ik}\partial_k \beta^j - \frac{2}{3}\bar{\gamma}^{ij}\partial_m \beta^m\right) \\
&= \partial_j \left(-2\alpha \bar{A}^{ij} - \beta^k \partial_k \bar{\gamma}^{ij} + 2\bar{\gamma}^{k(i}\partial_k \beta^{j)} - \frac{2}{3}\bar{\gamma}^{ij}\partial_k \beta^k\right).
\end{aligned} \tag{2.36}
$$

We may also rewrite (2.36) in terms of the coefficients $\bar{\Gamma}^i$, by using $\bar{\Gamma}^i = -\partial_j \bar{\gamma}^{ij}$:

$$
\begin{aligned}
\partial_t \bar{\Gamma}^i &= -2\partial_j(\alpha \bar{A}^{ij}) - \partial_j\left(\beta^k \partial_k \bar{\gamma}^{ij}\right) + \partial_j\left(\bar{\gamma}^{ki}\partial_k \beta^j\right) + \partial_j\left(\bar{\gamma}^{kj}\partial_k \beta^i\right) - \frac{2}{3}\partial_j\left(\bar{\gamma}^{ij}\partial_k \beta^k\right) \\
&= -2\alpha\partial_j \bar{A}^{ij} - 2\bar{A}^{ij}\partial_j \alpha - \beta^k \partial_k \underbrace{\partial_j \bar{\gamma}^{ij}}_{=-\bar{\Gamma}^i} \underbrace{-\partial_k \bar{\gamma}^{ij}\partial_j \beta^k}_{(\ddagger)} + \underbrace{\bar{\gamma}^{ki}\partial_k \partial_j \beta^j}_{(\dagger)} + \underbrace{\partial_j \bar{\gamma}^{ki}\partial_k \beta^j}_{=(\ddagger)\text{ by relabelling}} \\
&\quad + \bar{\gamma}^{kj}\partial_k \partial_j \beta^i + \underbrace{\partial_j \bar{\gamma}^{kj}}_{=-\bar{\Gamma}^k}\partial_k \beta^i - \frac{2}{3}\underbrace{\bar{\gamma}^{ij}\partial_j \partial_k \beta^k}_{=(\dagger)\text{ by relabelling}} - \frac{2}{3}\partial_k \beta^k \underbrace{\partial_j \bar{\gamma}^{ij}}_{=-\bar{\Gamma}^i} \\
&= -2\alpha\partial_j \bar{A}^{ij} - 2\bar{A}^{ij}\partial_j \alpha + \beta^j \partial_j \bar{\Gamma}^i + \bar{\gamma}^{jk}\partial_j \partial_k \beta^i - \bar{\Gamma}^j \partial_j \beta^i + \frac{1}{3}\bar{\gamma}^{ij}\partial_j \partial_k \beta^k + \frac{2}{3}\bar{\Gamma}^i \partial_j \beta^j.
\end{aligned} \tag{2.37}
$$

It may seem like we are now finally done deriving the evolution equations for all the BSSN variables listed on (2.1); however, we are still missing one crucial step! As it turns out, if we use the evolution equation for $\bar{\Gamma}^i$ in the form presented on Eq. (2.37), the whole system is numerically unstable (even more unstable than the ADM system we presented in Chapter 1!). To fix this, we need to expand the divergence of $\bar{A}_{ij}$ (first term on the RHS of Eq. (2.37)), with the aid of the momentum constraints. First recall the momentum constraints written in ADM form (c.f., Eq. 1.53),

$$
D_j\left(K^{ij} - \gamma^{ij}K\right) = 8\pi S^i.
$$

Now raising indices on Eq. (2.12) and inserting into this expression, we get

$$
D_j\left(A^{ij} - \frac{2}{3}\gamma^{ij}K\right) = 8\pi S^i. \tag{2.38}
$$

In order to expand this further, we will need the following result: using Eq. (2.31),

$$
\begin{aligned}
D_j \bar{A}^{ij} &= \partial_j \bar{A}^{ij} + \Gamma^i_{jk}\bar{A}^{jk} + \Gamma^j_{jk}\bar{A}^{ik} \\
&= \partial_j \bar{A}^{ij} + \left[\bar{\Gamma}^i_{jk} - \frac{1}{2}\chi^{-1}\left(\delta^i{}_k\,\partial_j \chi + \delta^i{}_j\,\partial_k \chi - \bar{\gamma}_{jk}\bar{\gamma}^{i\ell}\,\partial_\ell \chi\right)\right]\bar{A}^{jk} \\
&\qquad + \left[\bar{\Gamma}^j_{jk} - \frac{1}{2}\chi^{-1}\left(\delta^j{}_k\,\partial_j \chi + \delta^j{}_j\,\partial_k \chi - \bar{\gamma}_{jk}\bar{\gamma}^{j\ell}\,\partial_\ell \chi\right)\right]\bar{A}^{ik} \\
&= \underbrace{\partial_j \bar{A}^{ij} + \bar{\Gamma}^i_{jk}\bar{A}^{jk} + \bar{\Gamma}^j_{jk}\bar{A}^{ik}}_{=\bar{D}_j \bar{A}^{ij}} - \frac{1}{2}\chi^{-1}\left(\bar{A}^{ij}\,\partial_j \chi + \bar{A}^{ik}\,\partial_k \chi + \bar{A}^{ij}\,\partial_j \chi + 3\,\bar{A}^{ik}\partial_k \chi - \bar{A}^{ik}\partial_k \chi\right) \\
&= \bar{D}_j \bar{A}^{ij} - \frac{5}{2}\chi^{-1}\,\bar{A}^{ij}\,\bar{D}_j \chi.
\end{aligned}
$$

Now we plug this back into (2.38) and expand,

$$
\begin{aligned}
D_j A^{ij} - \frac{2}{3}\gamma^{ij}D_j K &= 8\pi S^i \\
D_j(\chi \bar{A}^{ij}) - \frac{2}{3}\chi\bar{\gamma}^{ij}\bar{D}_j K &= 8\pi S^i \\
\chi\, D_j \bar{A}^{ij} + \bar{A}^{ij}D_j \chi - \frac{2}{3}\chi \bar{D}^i K &= 8\pi S^i \\
\chi\left(\bar{D}_j \bar{A}^{ij} - \frac{5}{2}\chi^{-1}\,\bar{A}^{ij}\,\bar{D}_j \chi\right) + \bar{A}^{ij}D_j \chi - \frac{2}{3}\chi \bar{D}^i K &= 8\pi S^i.
\end{aligned}
$$

Writing $\bar{S}^i \equiv \chi^{-1}S^i$ $(= \chi^{-1}\gamma^{ij}S_j = \bar{\gamma}^{ij}S_j)$, we have our final expression for the momentum constraints in BSSN form:

$$
\boxed{\bar{D}_j \bar{A}^{ij} - \frac{3}{2\chi}\bar{A}^{ij}\,\bar{D}_j \chi - \frac{2}{3}\bar{D}^i K = 8\pi \bar{S}^i.} \tag{2.39}
$$

Note, however, that writing the full conformal covariant divergence on the first term on the LHS of Eq. (2.39) is unnecessary, since

$$\bar{D}_j\bar{A}^{ij} = \partial_j\bar{A}^{ij} + \bar{\Gamma}^i_{jk}\bar{A}^{jk} + \bar{\Gamma}^j_{jk}\bar{A}^{ik},$$

but

$$\bar{\Gamma}^j_{jk} = \frac{1}{2}\bar{\gamma}^{j\ell}\partial_k\bar{\gamma}_{j\ell} = \partial_k \log\sqrt{\bar{\gamma}} = 0,$$

where we used (yet again) Jacobi's formula, as well as the fact that we are working in Cartesian coordinates where $\bar{\gamma} = 1$. Hence, the conformal covariant divergence of $\bar{A}^{ij}$ simplifies to

$$\bar{D}_j\bar{A}^{ij} = \partial_j\bar{A}^{ij} + \bar{\Gamma}^i_{jk}\bar{A}^{jk}.$$

Now we isolate $\partial_j\bar{A}^{ij}$ on Eq. (2.39),

$$\partial_j\bar{A}^{ij} = \frac{3}{2\chi}\bar{A}^{ij}\,\bar{D}_j\chi + \frac{2}{3}\bar{D}^iK + 8\pi\bar{S}^i - \bar{\Gamma}^i_{jk}\bar{A}^{jk},$$

and insert back into Eq. (2.37) to arrive at our sought-after evolution equation for the coefficients $\bar{\Gamma}^i$:

$$\boxed{\begin{aligned}\partial_t\bar{\Gamma}^i = -2\alpha\left(\frac{3}{2\chi}\bar{A}^{ij}\,\bar{D}_j\chi + \frac{2}{3}\bar{D}^iK + 8\pi\bar{S}^i - \bar{\Gamma}^i_{jk}\bar{A}^{jk}\right) - 2\bar{A}^{ij}\bar{D}_j\alpha \\ + \beta^j\partial_j\bar{\Gamma}^i + \bar{\gamma}^{jk}\partial_j\partial_k\beta^i - \bar{\Gamma}^j\partial_j\beta^i + \frac{2}{3}\bar{\Gamma}^i\partial_j\beta^j + \frac{1}{3}\bar{\gamma}^{ij}\partial_j\partial_k\beta^k.\end{aligned}} \tag{2.40}$$

The last matter to take care of before we complete our presentation of the BSSN formalism is to also rewrite the Hamiltonian constraint in BSSN form; recall from Eq. (1.48),

$$R + K^2 - K_{ij}K^{ij} = 16\pi\rho.$$

From Eqs. (2.15) and (2.16), we have

$$\begin{aligned}K_{ij}K^{ij} &= \left[\chi^{-1}\left(\bar{A}_{ij} + \frac{1}{3}\bar{\gamma}_{ij}K\right)\right]\left[\chi\left(\bar{A}^{ij} + \frac{1}{3}\bar{\gamma}^{ij}K\right)\right] \\ &= \bar{A}_{ij}\bar{A}^{ij} + \frac{1}{3}K^2,\end{aligned} \tag{2.41}$$

where we used the tracelessness of $\bar{A}_{ij}$. We now plug this as well as the transformation law for the spatial Ricci scalar R (which is derived in full detail on Appendix B (c.f., Eq. (B.13))) into the Hamiltonian constraint:

$$\chi\bar{R} + 2\,\chi\bar{D}^2(\log\chi) - \frac{1}{2}\,\chi\bar{D}_k(\log\chi)\bar{D}^k(\log\chi) + K^2 - \bar{A}_{ij}\bar{A}^{ij} + \frac{1}{3}K^2 = 16\pi\rho$$
$$\chi\bar{R} + 2\,\chi\bar{D}^2(\log\chi) - \frac{1}{2}\,\chi\bar{D}_k(\log\chi)\bar{D}^k(\log\chi) + \frac{4}{3}K^2 - \bar{A}_{ij}\bar{A}^{ij} = 16\pi\rho.$$

Writing $\bar{\rho}^i \equiv \chi^{-1}\rho$, we have our final expression for the Hamiltonian constraint in BSSN form:

$$\boxed{\bar{R} + 2\,\bar{D}^2(\log\chi) - \frac{1}{2}\bar{D}_k(\log\chi)\bar{D}^k(\log\chi) + \frac{4}{3\chi}K^2 - \frac{1}{\chi}\bar{A}_{ij}\bar{A}^{ij} = 16\pi\bar{\rho}.} \tag{2.42}$$

Equations (2.42) and (2.39) are the Hamiltonian and momentum constraints, respectively, in BSSN variables. We shall not use them in this form, however, when solving the initial data problem in the next chapter, since more suitable conformal scalings will be used there.

This concludes our presentation of the BSSN formalism of numerical general relativity. Admittedly, this formalism is not nearly as intuitive and straightforward as the ADM alternative that we presented on the previous chapter, but it is nevertheless a much more robust formulation (from a numerical perspective).

This is a running theme in physics (and science in general): analytical and numerical implementations rarely play fair ball with each other. The ADM formalism is important for historical (and pedagogical) reasons, but it is nearly useless for practical purposes. We remark, however, that BSSN is not by any means the only modern successful approach to numerical relativistic studies; other flourishing alternatives such as the *Generalized Harmonic Coordinates with Constraint Damping* (GHCD) ([17], [21], [22]) and $Z4$-like formalisms ([3], [8], [10], [9], [24]) are just as good as (and in some cases even superior to) BSSN.

BSSN Equations

※ Evolution Equations:

$$\boxed{\begin{aligned}
\partial_t \chi &= \frac{2}{3}\chi(\alpha K - \partial_i\beta^i) + \beta^i \bar{D}_i\chi \\
\partial_t \bar{\gamma}_{ij} &= -2\alpha\bar{A}_{ij} + 2\bar{D}_{(i}\beta_{j)} - \frac{2}{3}\bar{\gamma}_{ij}\bar{D}_k\beta^k \\
\partial_t K &= \alpha\left(\bar{A}_{ij}\bar{A}^{ij} + \frac{1}{3}K^2\right) + 4\pi\alpha(\rho + S) - D^2\alpha + \beta^i\bar{D}_i K \\
\partial_t \bar{A}_{ij} &= \left[\chi(\alpha R_{ij} - 8\pi\alpha S_{ij} - D_iD_j\alpha)\right]^{\mathrm{TF}} - \alpha(2\bar{A}_{ik}\bar{A}^k{}_j + \bar{A}_{ij}K) \\
&\quad + \beta^k\partial_k\bar{A}_{ij} + \bar{A}_{ik}\partial_j\beta^k + \bar{A}_{kj}\partial_i\beta^k - \frac{2}{3}\bar{A}_{ij}\partial_k\beta^k \\
\partial_t\bar{\Gamma}^i &= -2\alpha\left(\frac{3}{2\chi}\bar{A}^{ij}\,\bar{D}_j\chi + \frac{2}{3}\bar{D}^iK + 8\pi\bar{S}^i - \bar{\Gamma}^i_{jk}\bar{A}^{jk}\right) - 2\bar{A}^{ij}\bar{D}_j\alpha \\
&\quad + \beta^j\partial_j\bar{\Gamma}^i + \bar{\gamma}^{jk}\partial_j\partial_k\beta^i - \bar{\Gamma}^j\partial_j\beta^i + \frac{2}{3}\bar{\Gamma}^i\partial_j\beta^j + \frac{1}{3}\bar{\gamma}^{ij}\partial_j\partial_k\beta^k
\end{aligned}}$$

In these equations we need to rewrite the (second) spatial derivatives of the lapse as

$$\boxed{D_iD_j\alpha = \bar{D}_i\bar{D}_j\alpha + \frac{1}{2\chi}\left(2\bar{D}_{(i}\chi\bar{D}_{j)}\alpha - \bar{\gamma}_{ij}\,\bar{D}_k\chi\,\bar{D}^k\alpha\right)}$$

Also the Ricci tensor is split as

$$\boxed{\begin{aligned}
R_{ij} &= \bar{R}_{ij} + R^{\chi}_{ij} \\
\bar{R}_{ij} &= -\frac{1}{2}\bar{\gamma}^{k\ell}\partial_k\partial_\ell\bar{\gamma}_{ij} + \bar{\gamma}_{k(i}\partial_{j)}\,\bar{\Gamma}^k + \bar{\Gamma}^k\,\bar{\Gamma}_{(ij)k} + \bar{\gamma}^{k\ell}\left(2\,\bar{\Gamma}^m_{k(i}\bar{\Gamma}_{j)m\ell} + \bar{\Gamma}^m_{ik}\,\bar{\Gamma}_{j\ell m}\right) \\
R^{\chi}_{ij} &= \frac{1}{2}\left(\bar{D}_i\bar{D}_j(\log\chi) + \bar{\gamma}_{ij}\,\bar{D}_k\bar{D}^k(\log\chi)\right) \\
&\quad + \frac{1}{4}\left(\bar{D}_i(\log\chi)\bar{D}_j(\log\chi) - \bar{\gamma}_{ij}\,\bar{D}_k(\log\chi)\bar{D}^k(\log\chi)\right)
\end{aligned}}$$

※ Constraint Equations:

$$\boxed{\begin{aligned}
\bar{R} + 2\,\bar{D}^2(\log\chi) - \frac{1}{2}\bar{D}_k(\log\chi)\bar{D}^k(\log\chi) + \frac{4}{3\chi}K^2 - \frac{1}{\chi}\bar{A}_{ij}\bar{A}^{ij} &= 16\pi\bar{\rho} \\
\bar{D}_j\bar{A}^{ij} - \frac{3}{2\chi}\bar{A}^{ij}\,\bar{D}_j\chi - \frac{2}{3}\bar{D}^iK &= 8\pi\bar{S}^i
\end{aligned}}$$

Part II

The Model: Bowen-York Black Hole Data

3

The Initial Data Problem

As we have alluded to earlier, we are not free to impose whatever data we like on our hypersurfaces; the initial data has to be chosen in such a way that the Hamiltonian (c.f., Eq. (1.48)) and momentum (c.f., Eq. (1.53)) constraints are satisfied from the onset and remain satisfied throught the entire time-evolution of the system. It can be shown (analytically, via the Bianchi identities) that if the constraints are satisfied on some initial time slice, they will remain fulfilled for the entirety of the simulation. This is, however, an *analytical* statement; in *numerical* simulations the constraints will be violated, and this is something that needs to be monitored. In practice, some sort of damping technique is applied to keep these violations in check. However, our concern in this work is exclusively on the *initial data*. The evolution of the EFEs, which are given by the BSSN equations presented in the previous chapter, will not be discussed any further in this treatment.

Let us recall what the constraint equations look like (in ADM form). In fact, since our focus will be exclusively on *black hole data*, we shall ignore matter terms and rewrite these equations in the vacuum:

$$R + K^2 - K^{ij}K_{ij} = 0; \qquad \text{(Hamiltonian)} \tag{3.1a}$$

$$D_j\left(K^{ij} - \gamma^{ij}K\right) = 0. \qquad \text{(Momentum)} \tag{3.1b}$$

The first thing we note is that we only have four equations (one for the Hamiltonian; three for the momentum), but twelve unknowns $\{\gamma_{ij}, K_{ij}\}$. Thus the system is underdetermined. Moreover, the operator R (Ricci scalar) in the Hamiltonian is a fairly complicated operator that is not ideal to work with. In an effort to somewhat mitigate these problems, we introduce (yet again) a conformal rescaling of the quantities involved. This was the approach originally taken by Lichnerowicz [18] and York [27], and it is widely used in the NR community to this day.

Thus we start with the conformal rescaling for the metric

$$\boxed{\begin{aligned} \gamma_{ij} &= \psi^4\bar{\gamma}_{ij} \qquad (3.2\text{a}) \\ \gamma^{ij} &= \psi^{-4}\bar{\gamma}^{ij}. \qquad (3.2\text{b}) \end{aligned}}$$

The specific power that we chose for the conformal factor ψ is not relevant at all from a theoretical perspective; it is merely chosen for convenience for certain calculations. The only quantity here that has *physical* meaning is the spatial metric γ_{ij}, which we can always recover via Eqs. (3.2), regardless of what particular power we choose for the scaling factor. Another quantity that will have a different scaling now is the traceless curvature A_{ij}; let us see why it is convenient to use a different factor for the latter: Start by putting

$$A^{ij} = \psi^{\eta}\widetilde{A}^{ij}, \tag{3.3}$$

where η is some user-defined constant. Note that we have now replaced the bar with a tilde (and we will do so throughout this chapter) to differentiate from the *Nakamura* rescaling of A_{ij} introduced in the BSSN formalism (c.f., Eq. (2.13)) which, in terms of ψ, would equate to $\eta = -4$. Now note that Eq. (3.1b) can be written as

$$D_j K^{ij} = D^i K.$$

From Eq. (2.12) we can then rewrite this expression as

$$D_j \left(A^{ij} + \frac{1}{3}\gamma^{ij} K \right) = D^i K \quad \Longrightarrow \quad D_j A^{ij} = \frac{2}{3} D^i K. \tag{3.4}$$

We now expand the divergence of A_{ij} in terms of the conformal connection $\bar{D}$, using (B.11) and applying it on Eq. (B.1) (see Appendix B):

$$\begin{aligned}
D_j A^{ij} &= \bar{D}_j A^{ij} + A^{kj}\mathfrak{C}^i{}_{jk} + A^{ik}\mathfrak{C}^j{}_{jk} \\
&= \bar{D}_j A^{ij} + A^{kj}\left[4\delta_{(j}{}^{i}\,\bar{D}_{k)}(\log\psi) - 2\bar{\gamma}_{jk}\,\bar{D}^i(\log\psi)\right] \\
&\qquad + A^{ik}\left[4\delta_{(j}{}^{j}\,\bar{D}_{k)}(\log\psi) - 2\bar{\gamma}_{jk}\,\bar{D}^j(\log\psi)\right] \\
&= \bar{D}_j A^{ij} + 2A^{ik}\bar{D}_k(\log\psi) + 2A^{ij}\bar{D}_j(\log\psi) - 2A^{kj}\bar{\gamma}_{jk}\,\bar{D}^i(\log\psi) \\
&\qquad + 6A^{ik}\bar{D}_k(\log\psi) + 2A^{ij}\bar{D}_j(\log\psi) - 2A^{ik}\,\bar{D}_k(\log\psi) \\
&= \bar{D}_j A^{ij} + 10A^{ij}\bar{D}_j(\log\psi) - 2A^{jk}\bar{\gamma}_{jk}\,\bar{D}^i(\log\psi) \\
&= \bar{D}_j A^{ij} + 10A^{ij}\bar{D}_j(\log\psi) - 2\psi^{-4}\underbrace{A^{jk}\gamma_{jk}}_{=0}\,\bar{D}^i(\log\psi) \\
&= \bar{D}_j A^{ij} + 10A^{ij}\bar{D}_j(\log\psi).
\end{aligned}$$

This result can be rewritten as

$$D_j A^{ij} = \psi^{-10}\bar{D}_j\left(\psi^{10}A^{ij}\right), \tag{3.5}$$

which suggests that we define the quantity

$$\widetilde{A}^{ij} = \psi^{10}A^{ij}, \tag{3.6}$$

which corresponds to setting $\eta = -10$ on Eq. (3.3). This rescaling of A_{ij}, which was first introduced by Lichnerowicz [18], will be the one used when solving the constraints on the initial data; we shall call it the *Lichnerowicz scaling of A_{ij}*. Lowering indices on Eq. (3.6) we find [1]

$$\begin{aligned}
\gamma_{ik}\gamma_{j\ell}A^{ij} &= \psi^{-10}\widetilde{A}^{ij}\gamma_{ik}\gamma_{j\ell} \\
A_{k\ell} &= \psi^{-10}\widetilde{A}^{ij}\,\psi^4\bar{\gamma}_{ik}\,\psi^4\bar{\gamma}_{j\ell} \\
A_{k\ell} &= \psi^{-2}\widetilde{A}_{k\ell}.
\end{aligned}$$

In summary,

$$\boxed{\begin{aligned} A_{ij} &= \psi^{-2}\widetilde{A}_{ij} \qquad (3.7a)\\ A^{ij} &= \psi^{-10}\widetilde{A}^{ij}. \qquad (3.7b)\end{aligned}}$$

Now, from (3.1b) and (3.4)–(3.6), we get

$$\begin{aligned}
D_j A^{ij} - \frac{2}{3}\gamma^{ij}D_j K &= 0 \\
\psi^{-10}\bar{D}_j\widetilde{A}^{ij} - \frac{2}{3}\psi^{-4}\bar{\gamma}^{ij}\bar{D}_j K &= 0 \\
\bar{D}_j\widetilde{A}^{ij} - \frac{2}{3}\psi^{6}\bar{D}^i K &= 0.
\end{aligned}$$

[1]Note that A_{ij} may have a different scaling factor, but it is still a quantity related to the conformal metric $\bar{\gamma}_{ij}$, so indices of $\widetilde{A}_{ij}$ shall be raised/lowered with $\bar{\gamma}_{ij}$.

Hence we have our momentum constraints in the vacuum:

$$\boxed{\bar{D}_j \widetilde{A}^{ij} - \frac{2}{3}\psi^6 \bar{D}^i K = 0.} \tag{3.8}$$

Lastly, we need the Hamiltonian. Recall from Eq. (2.41) that

$$K_{ij}K^{ij} = \bar{A}_{ij}\bar{A}^{ij} + \frac{1}{3}K^2,$$

where $\bar{A}_{ij}$ is the Nakamura scaling of A_{ij}. Rewriting the first term on the RHS in terms of the Lichnerowicz scaling,

$$\bar{A}_{ij}\bar{A}^{ij} = \psi^4\psi^{-4}A_{ij}A^{ij} = A_{ij}A^{ij} = \psi^{-2}\psi^{-10}\widetilde{A}_{ij}\widetilde{A}^{ij} = \psi^{-12}\widetilde{A}_{ij}\widetilde{A}^{ij}, \tag{3.9}$$

and plugging in the transformation law for the spatial Ricci scalar R (which is derived in full detail on Appendix B (c.f., Eq. B.13)) in terms of ψ instead of χ,

$$R = \psi^{-4}\bar{R} - 8\psi^{-5}\bar{D}^2\psi,$$

we get (in the vacuum)

$$\begin{aligned} R + K^2 - K_{ij}K^{ij} &= 0 \\ \psi^{-4}\bar{R} - 8\psi^{-5}\bar{D}^2\psi + \frac{2}{3}K^2 - \psi^{-12}\widetilde{A}_{ij}\widetilde{A}^{ij} &= 0 \\ \bar{D}^2\psi + \frac{1}{8}\left(\psi^{-7}\widetilde{A}_{ij}\widetilde{A}^{ij} - \psi\bar{R}\right) - \frac{1}{12}\psi^5 K^2 &= 0. \end{aligned}$$

Thus we have our (vacuum) Hamiltonian constraint in its final (Lichnerowicz) form:

$$\boxed{\bar{D}^2\psi + \frac{1}{8}\left(\psi^{-7}\widetilde{A}_{ij}\widetilde{A}^{ij} - \psi\bar{R}\right) - \frac{1}{12}\psi^5 K^2 = 0.} \tag{3.10}$$

3.1. Conformal Transverse-Traceless (CTT) Decomposition

Most known decompositions of the initial data problem start with the Lichnerowicz-York conformal transformations introduced above; from this point on the different approaches (such as the one introduced in this section) proceed to decompose the (rescaled) traceless extrinsic curvature $\widetilde{A}^{ij}$ in different ways. For the *conformal transverse-traceless* (CTT) decomposition, we start by splitting $\widetilde{A}^{ij}$ as [2]

$$\widetilde{A}^{ij} = \widetilde{A}^{ij}_{\mathrm{L}} + \widetilde{A}^{ij}_{\mathrm{TT}} = (\bar{\mathbb{L}}\boldsymbol{X})^{ij} + \widetilde{A}^{ij}_{\mathrm{TT}}, \tag{3.11}$$

where $\widetilde{A}^{ij}_{\mathrm{TT}}$ is the *transverse-traceless* (TT) part of $\widetilde{A}^{ij}$:

$$\bar{D}_j \widetilde{A}^{ij}_{\mathrm{TT}} = 0 \qquad (\text{Transverse}) \tag{3.12a}$$

$$\bar{\gamma}_{ij}\widetilde{A}^{ij}_{\mathrm{TT}} = 0. \qquad (\text{Traceless}) \tag{3.12b}$$

On the other hand, the *longitudinal* (L) part of $\widetilde{A}^{ij}$, namely $\widetilde{A}^{ij}_{\mathrm{L}}$, is expressed in terms of the *conformal Killing operator* $(\bar{\mathbb{L}}\boldsymbol{X})^{ij}$ associated with the conformal metric $\bar{\gamma}_{ij}$ and some vector field $\boldsymbol{X}$,

$$\boxed{(\bar{\mathbb{L}}\boldsymbol{X})^{ij} \equiv 2\bar{D}^{(i}X^{j)} - \frac{2}{3}\bar{\gamma}^{ij}\bar{D}_k X^k.} \tag{3.13}$$

[2] In fact, it can be shown that *any* symmetric, trace-free tensor can be split into a sum of its transverse/orthogonal/divergence-free part and its longitudinal part, the latter being given by the Killing operator, as in (3.13).

The vector field $\boldsymbol{X}$ is determined from taking the divergence of (3.11)

$$\bar{D}_j(\bar{\mathbb{L}}\boldsymbol{X})^{ij} = \bar{D}_j\widetilde{A}^{ij}, \tag{3.14}$$

where we used the transverse property (3.12a). This second-order operator is crucial to our work, so we shall give it its own unique notation:

$$\bar{\Delta}_{\bar{\mathbb{L}}}X^i \equiv \bar{D}_j(\bar{\mathbb{L}}\boldsymbol{X})^{ij}. \tag{3.15}$$

Expanding,

$$\begin{aligned}
\bar{\Delta}_{\bar{\mathbb{L}}}X^i = \bar{D}_j(\bar{\mathbb{L}}\boldsymbol{X})^{ij} &= \bar{D}_j\left(\bar{D}^iX^j + \bar{D}^jX^i - \frac{2}{3}\bar{\gamma}^{ij}\bar{D}_kX^k\right)\\
&= \underbrace{\bar{D}_j\bar{D}^iX^j}_{=\bar{R}^i{}_jX^j+\bar{D}^i\bar{D}_jX^j} + \bar{D}^2X^i - \frac{2}{3}\bar{D}^i\bar{D}_jX^j\\
&= \bar{D}^2X^i + \bar{R}^i{}_jX^j + \frac{1}{3}\bar{D}^i\bar{D}_jX^j. && \text{(by Ricci identity)}
\end{aligned}$$

Thus we have the *conformal vector Laplacian*

$$\boxed{\bar{\Delta}_{\bar{\mathbb{L}}}X^i = \bar{D}^2X^i + \bar{R}^i{}_jX^j + \frac{1}{3}\bar{D}^i\bar{D}_jX^j.} \tag{3.16}$$

From (3.14) we see that the existence and uniqueness of the L-TT decomposition (3.11) is guaranteed if and only if there exists a unique solution X^i to Eq. (3.16). We shall now rewrite the momentum constraints using this conformal Laplacian operator: from Eqs. (3.14)–(3.15), we see that Eq. (3.8) becomes

$$\boxed{\bar{\Delta}_{\bar{\mathbb{L}}}X^i - \frac{2}{3}\psi^6\bar{D}^iK = 0.} \tag{3.17}$$

Thus we have reduced the Hamiltonian and momentum constraints to equations that need to be solved for ψ and X^i, respectively. Note that the second term on the LHS of Eq. (3.17) couples the constraints; under the assumption that $K =$ constant (e.g., the *maximal slicing* condition $K = 0$) they decouple. In such situations we can first solve Eq. (3.17) for X^i, from which we determine $\widetilde{A}^{ij}$, which we then plug into Eq. (3.10) and solve the Hamiltonian constraint for ψ. This is precisely the approach we shall take in the *Bowen-York* solutions, discussed in the following section. Once we have the solutions, we then need to recover the *physical* data from it: from ψ we recover $\bar{\gamma}_{ij}$ and, accordingly, γ_{ij}; from X^i we recover $\widetilde{A}^{ij}$ via (3.14) (consequently A_{ij} and, ultimately, the physical data K_{ij}).

Let us briefly recap the situation. We start off with twelve degrees of freedom (DoF) in the physical system $\{\gamma_{ij}, K_{ij}\}$, four of which are removed due to the constraints (one is the conformal factor ψ from the Hamiltonian (3.10); three come from X^i or, equivalently, the longitudinal part of the extrinsic curvature $\widetilde{A}^{ij}_{\mathrm{L}} = (\bar{\mathbb{L}}\boldsymbol{X})^{ij}$ which is recovered from the momentum constraints (3.17)). A further four DoF account for the gauge freedom that is inherent to GR (three spatial coordinates associated with the physical 3-metric γ_{ij} and a time coordinate that is associated with K). Hence from the initial twelve DoF we are left with only four that are still undetermined:

- ⋇ (Two undetermined DoF in the conformal metric, $\bar{\gamma}_{ij}$) From the possible six DoF of $\bar{\gamma}_{ij}$, one is lost once we fix the conformal factor ψ while other three are due to the spatial-coordinate freedom. In other words, there are actually five DoF encoded in $\bar{\gamma}_{ij}$, albeit only two of them are true dynamical degrees of freedom of the gravitational field;
- ⋇ (Two undetermined DoF in the TT part of the extrinsic curvature, $\widetilde{A}^{ij}_{\mathrm{TT}}$) From the possible six DoF of $\widetilde{A}^{ij}_{\mathrm{TT}}$, one is lost due to the traceless property (3.12b) and three more due to the transverse property (3.12a).

These four are the true dynamical DoF of the gravitational field; the remaining eight are either fixed by constrains (four) or represent gauge freedom (four). All in all, the CTT approach puts as *constrained data* the quantities ψ and X^i whilst leaving as *free data* the quantities $\{\widetilde{A}^{ij}_{\mathrm{TT}}, \bar{\gamma}_{ij}, K\}$. The choice of this *free background data* has to be made according to the physical meaning of the scenario one would like to present (e.g., black holes, neutron stars, exotic compacts, etc). We shall see in the next section a commonly used choice of free data for the construction of black holes.

CTT Decomposition

In the CTT approach, initial data is split as follows

- Constrained Data: ψ, X^i;
- Free Data: $\widetilde{A}^{ij}_{\mathrm{TT}}, \bar{\gamma}_{ij}, K$.

The Hamiltonian constraint is

$$\boxed{\bar{D}^2\psi + \frac{1}{8}\left(\psi^{-7}\widetilde{A}_{ij}\widetilde{A}^{ij} - \psi\bar{R}\right) - \frac{1}{12}\psi^5 K^2 = 0}$$

where $\widetilde{A}^{ij}$ is given by

$$\widetilde{A}^{ij} = \widetilde{A}^{ij}_{\mathrm{L}} + \widetilde{A}^{ij}_{\mathrm{TT}} = (\bar{\mathbb{L}}\boldsymbol{X})^{ij} + \widetilde{A}^{ij}_{\mathrm{TT}}.$$

It needs to be solved for ψ. On the other hand, the momentum constraints are

$$\boxed{\bar{\Delta}_{\mathbb{L}} X^i - \frac{2}{3}\psi^6 \bar{D}^i K = 0}$$

which need to be solved for X^i.

The physical solution is then constructed from

$$\gamma_{ij} = \psi^4 \bar{\gamma}_{ij}$$
$$K_{ij} = \psi^{-2}\widetilde{A}_{ij} + \frac{1}{3}\gamma_{ij}K.$$

3.2. Bowen-York Solutions

In the Bowen-York (BY) approach [11], only the Hamiltonian will need to be solved numerically; the momentum constraints simplify in such a way that a closed-form solution is possible. These solutions are built up from the CTT framework discussed in the previous section. We recall that the free (unconstrained) data in this formalism are the quantities $\widetilde{A}^{ij}_{\mathrm{TT}}$, $\bar{\gamma}_{ij}$, and K. In BY the following choices are made:

$$\widetilde{A}^{ij}_{\mathrm{TT}} = 0 \tag{3.18a}$$
$$K = 0 \tag{3.18b}$$
$$\bar{\gamma}_{ij} = f_{ij}, \tag{3.18c}$$

where f_{ij} is the flat metric ($= \delta_{ij}$ in Cartesian coordinates); Eq. (3.18c) is the *conformally-flat condition* imposed on the spatial metric. Eq. (3.18b) is called the *maximal slicing condition*; the name comes from the fact that a spatial hypersurface that satisfies $K = 0$ has volume that can be shown to be extremal (which, in the case of a Lorentzian metric, is maximal). The role of the relation (3.18a) is that now the extrinsic curvature will be completely determined by the longitudinal part $\widetilde{A}^{ij}_{\mathrm{L}}$ (c.f., eq. (3.11)).

Hence, due to the maximal slicing condition $K = 0$, the momentum constraints become

$$\bar{\Delta}_{\mathbb{L}} X^i = 0. \tag{3.19}$$

Moreover, since $\bar{\gamma}_{ij}$ is flat, its associated Ricci tensor $\bar{R}_{ij}$ vanishes and, since we are using Cartesian coordinates, all flat covariant derivatives become partial derivatives (i.e., $\bar{D}_i = \partial_i$). Whence we may expand Eq. (3.19) as follows (c.f., Eq. (3.16)):

$$\boxed{\partial^2 X^i + \frac{1}{3}\,\partial^i \partial_j X^j = 0.} \tag{3.20}$$

Techniques to solve this vector Laplacian can be found in the literature (e.g., [6], [11]). The basic idea is to introduce an ansatz for X^i that simplifies Eq. (3.20) in such a way that only a Laplacian term remains and all other derivatives cancel. Two such solutions (the most useful for our purposes) are given by

$$X^i_{\vec{J}} = \frac{1}{r^2}\left(\bar{\epsilon}^{ijk}\,\ell_j J_k\right), \tag{3.21a}$$

$$X^i_{\vec{P}} = -\frac{1}{4r}\left(7P^i + \ell^i \ell_j P^j\right). \tag{3.21b}$$

Here P^i and J^i are vectors with constant entries; they will represent the *linear-* and *angular momenta*, respectively. The object $\bar{\epsilon}^{ijk}$ is the antisymmetric (Levi-Civita) tensor compatible with the conformal metric $\bar{\gamma}_{ij}$: it satisfies $\bar{D}_l \bar{\epsilon}^{ijk} = 0$. Lastly, $\ell^i = x^i/r$ is the outward unit radial vector that is normal to the Euclidean sphere with radius $r = \sqrt{(x^1)^2 + (x^2)^2 + (x^3)^2}$. We can now recover $\widetilde{A}^{ij}_{\mathrm{L}}$ ($= \widetilde{A}^{ij}$, since $\widetilde{A}^{ij}_{\mathrm{TT}} = 0$) from plugging either (or both) of the solutions (3.21) into the expression for the conformal Killing operator:

$$\widetilde{A}^{ij} = \widetilde{A}^{ij}_{\mathrm{L}} = (\bar{\mathbb{L}}\boldsymbol{X})^{ij} = 2\bar{D}^{(i}X^{j)} - \frac{2}{3}\,\bar{\gamma}^{ij}\bar{D}_k X^k.$$

This yields

$$\boxed{\begin{aligned} \widetilde{A}^{ij}_{\vec{J}} &= \frac{6}{r^3}\ell^{(i}\bar{\epsilon}^{j)kl}J_k\ell_l && (3.22a)\\ \widetilde{A}^{ij}_{\vec{P}} &= \frac{3}{2r^2}\left[2P^{(i}\ell^{j)} + \ell_k P^k\left(\ell^i\ell^j - \delta^{ij}\right)\right] && (3.22b)\end{aligned}}$$

depending on whether we use $X^i_{\vec{J}}$ or $X^i_{\vec{P}}$ from Eqs. (3.21). The curvatures $\widetilde{A}^{ij}_{\vec{J}}$ and $\widetilde{A}^{ij}_{\vec{P}}$ describe a rotating black hole with angular momentum $\vec{J}$ and a black hole with linear momentum $\vec{P}$, respectively. We can also study a black hole that has both linear and angular momenta, by considering

$$\boxed{\widetilde{A}^{ij}_{\pm} = \widetilde{A}^{ij}_{\vec{P}} \pm \widetilde{A}^{ij}_{\vec{J}}.} \tag{3.22c}$$

In our model we shall construct inital data for a single black hole that has both types of momenta.

3.3. Puncture Initial Data

As a consequence of using the maximal slicing condition $K = 0$, the Hamiltonian and momentum constraints decoupled. Thus the approach we take is to solve first the momentum constraints analytically (as described in the previous section) and then plug the resulting extrinsic curvature $\widetilde{A}^{ij}$ from Eqs. (3.22) into the Hamiltonian:

$$\partial^2\psi + \frac{1}{8}\psi^{-7}\widetilde{A}_{ij}\widetilde{A}^{ij} = 0. \tag{3.23}$$

This is a Poisson-type nonlinear equation that needs to be solved numerically. The key idea to solve this rather complicated elliptic PDE is to first consider its homogeneous counterpart

$$\partial^2\psi = 0. \tag{3.24}$$

One solution to (3.24) of particular relevance for NR was found by Dieter R. Brill and Richard W. Lindquist [13]; it is a (spherically symmetric, asymptotically flat) solution on $\mathbb{R}^3 \setminus \{0\}$ that represents a black hole momentarily at rest (i.e., a black hole that satisfies $K_{ij} = 0$):

$$\psi = 1 + \frac{M}{2r}, \tag{3.25}$$

where r is the isotropic radius (at $r = 0$ we have the singularity (or "puncture") that represents the black hole) and M is the ADM mass of the black hole (see, e.g., [6], exercise 3.20). This solution is none other than the Schwarzschild spacetime in isotropic coordinates:

$$\begin{aligned} dl^2 = \gamma_{ij}\mathrm{d}x^i\mathrm{d}x^j &= \psi^4\bar{\gamma}_{ij}\mathrm{d}x^i\mathrm{d}x^j \\ &= \left(1 + \frac{M}{2r}\right)^4 \delta_{ij}\mathrm{d}x^i\mathrm{d}x^j \\ &= \left(1 + \frac{M}{2r}\right)^4 \left(\mathrm{d}r^2 + r^2(\mathrm{d}\theta^2 + \sin^2\theta\mathrm{d}\phi^2)\right). \end{aligned}$$

Moreover, since the Laplace equation (3.24) is linear, a trivial extension of the solution (3.25) to multiple (say, N) black holes that are momentarily at rest is given by

$$\psi = 1 + \sum_i^N \frac{M_i}{2r_i}, \tag{3.26}$$

with r_i being the coordinate separation from the i^{th} black hole's centre and the total ADM mass of the system given by the sum of the coefficients M_i. [3] We stress, however, that this very simple solution is only made possible by the *moment-of-time symmetry* assumption $K_{ij} = 0$, which does not hold for more realistic, nonstatic black holes. Nevertheless, it serves as a foundation for the following elegant breakthrough, which was pioneered in the late 90's by Brandt & Brügmann [12]. Their idea to tackle the inhomogeneous, nonlinear equation (3.23) was to extend the solution (3.26) by introducing a correction term u:

$$\psi = 1 + \frac{1}{\vartheta} + u, \qquad \text{where} \quad \frac{1}{\vartheta} \equiv \sum_i^N \frac{M_i}{2r_i}. \tag{3.27}$$

Plugging this ansatz back into the Hamiltonian (3.23), and using the fact that $\vartheta \to 0$ at the punctures:

$$\begin{aligned} \partial^2\left(1 + \frac{1}{\vartheta} + u\right) + \frac{1}{8}\left(1 + \frac{1}{\vartheta} + u\right)^{-7} \widetilde{A}_{ij}\widetilde{A}^{ij} = 0 \\ \partial^2 u + \frac{1}{8\vartheta^{-7}}\left(\vartheta + 1 + u\vartheta\right)^{-7} \widetilde{A}_{ij}\widetilde{A}^{ij} = 0. \end{aligned}$$

Using the notation

$$\varrho \equiv \frac{\vartheta^7}{8}\widetilde{A}_{ij}\widetilde{A}^{ij}, \tag{3.28}$$

we end up with the final form of the Hamiltonian constraint:

$$\boxed{\partial^2 u = -\varrho\left(\vartheta(1+u) + 1\right)^{-7}.} \tag{3.29}$$

The whole point of solving for the correction term u is that this function "absorbs" the singularities and is thus smooth everywhere, unlike our ansatz ψ which was singular at the punctures.

[3] Note that only when considering large separations between the individual black holes in the system can we identify M_i as the mass associated with the i^{th} black hole, since otherwise nontrivial interactions between the black holes can contribute to the overall mass.

4

Numerical Methods, Results & Conclusions

In this concluding chapter we compute the Hamiltonian constraint (3.29) and discuss the results. We note that the equation is of the form

$$\partial^2 u = f(u), \qquad \text{where} \quad f(u) = -\varrho\left(\vartheta(1+u)+1\right)^{-7}. \tag{4.1}$$

Since this equation is nonlinear on u, our first step is to linearize. First let us define the *residual* at the n^{th}-step, $R^{[n]}$, which is given by

$$R^{[n]} \equiv \partial^2 u^{[n]} - f(u^{[n]}). \tag{4.2}$$

(the $[n]$ superscript will always denote the n^{th}-iteration in the algorithm.) We then write

$$u^{[n+1]} = u^{[n]} + \delta u, \qquad \text{with} \quad \delta u \ll u^{[n]}, \tag{4.3}$$

and Taylor-expand f to first order:

$$\begin{aligned} f(u^{[n+1]}) &= f(u^{[n]} + \delta u) \\ &= f(u^{[n]}) + f'(u^{[n]})\delta u + \mathcal{O}((\delta u)^2), \end{aligned} \tag{4.4}$$

where $f' = \mathrm{d}f/\mathrm{d}u$. Dropping higher-order terms and plugging $u^{[n+1]}$ into Eq. (4.1), we get

$$\begin{aligned} \partial^2(u^{[n+1]}) &= f(u^{[n+1]}) \\ \partial^2(u^{[n]} + \delta u) &= f(u^{[n]}) + f'(u^{[n]})\delta u \\ \partial^2(\delta u) - f'(u^{[n]})\delta u &= f(u^{[n]}) - \partial^2 u^{[n]}. \end{aligned}$$

Noting that the RHS is simply $-R^{[n]}$, we end up with

$$\boxed{\partial^2(\delta u) - f'(u^{[n]})\delta u = -R^{[n]},} \tag{4.5}$$

where

$$f'(u^{[n]}) = 7\varrho\vartheta\left(\vartheta(1+u^{[n]})+1\right)^{-8}. \tag{4.6}$$

Our code iterates Eq. (4.5) until the residual $R^{[n]}$ reaches some desired tolerance. The perturbation solution δu updates the correction term u (which is the one we are really after) at every iteration, per Eq. (4.3).

4.1. Discretization in Three Dimensions

We note that Eq. (4.5) is of the form

$$\partial^2\varphi + g\varphi = b. \tag{4.7}$$

In three dimensions, using equal grid-spacing $h \equiv \Delta x = \Delta y = \Delta z$ with the same number of grid-points N in every dimension, and using the usual discrete notation $\varphi_{ijk} = \varphi(x_i, y_j, z_k)$, we have (using centered difference for the Laplace operator ∂^2)

$$\varphi_{i-1,j,k} + \varphi_{i,j-1,k} + \varphi_{i,j,k-1} + \left(h^2 g_{ijk} - 6\right)\varphi_{ijk} + \varphi_{i+1,j,k} + \varphi_{i,j+1,k} + \varphi_{i,j,k+1} = h^2 b_{ijk}, \tag{4.8}$$

for the initerior points $1 \le i, j, k \le N-1$ (we shall discuss the boundary conditions in a moment). The idea then is to use a *superindex* I, given by

$$I = i + Nj + N^2 k, \tag{4.9}$$

that sweeps across the 3D grid. Using the notation

$$\Phi_I = \varphi_{ijk}, \quad \Phi_{I\pm 1} = \varphi_{i\pm 1,j,k}, \quad \Phi_{I\pm N} = \varphi_{i,j\pm 1,k}, \quad \Phi_{I\pm N^2} = \varphi_{i,j,k\pm 1}$$

and, similarly, $G_I = g_{ijk}$ and $B_I = b_{ijk}$, Eq. (4.8) becomes

$$\Phi_{I-1} + \Phi_{I-N} + \Phi_{I-N^2} + \left(h^2 G_I - 6\right)\Phi_I + \Phi_{I+1} + \Phi_{I+N} + \Phi_{I+N^2} = h^2 B_I \tag{4.10}$$

which, again, only holds for values of I that correspond to $1 \le i, j, k \le N-1$. That brings us to the boundary conditions: as typical in GR, when dealing with a compact, isolated object (e.g., a star or a black hole), we would like to impose *asymptotic flatness*. This means that as we move far away from the object, the metric tensor becomes flat (that is, $\lim_{r\to\infty}\gamma_{ij}(r) = f_{ij}$). The only way this happens in our case is if $\psi \to 1$ as $r \to \infty$; looking back at Eq. (3.27) we see that $1/\vartheta \to 0$ as $r \to \infty$, so the only term that we must make sure also vanishes is the correction function u. To that end, we may impose the Robin condition at the boundaries

$$\partial_r(ru) = 0. \tag{4.11}$$

Discretizing in three dimensions, using the superindex I and writing $\Phi = u$, we get the Robin boundary conditions that cover the points that were excluded from Eq. (4.10). For instance, for the upper y-boundary, where $j = N-1$:

$$r_{ijk}\Phi_I - r_{i,j-1,k}\Phi_{I-N} = 0,$$

and similarly for the remaining boundaries. We are now finally ready to start writing the code; comparing Eqs. (4.5) and (4.7), we see that we must substitute $\varphi = \delta u$, $g = -f'(u^{[n]})$, and $b = -R^{[n]}$. Before proceeding with the code, however, we note that the matrix of coefficients of Eq. (4.10) is a band-diagonal matrix (seven bands) which can get very large; it is an $N^3 \times N^3$ matrix, so it contains N^6 elements. We thus need to either use sparse allocation to exploit its band-diagonal structure, or simply work with a somewhat coarse resolution. [1]

4.2. Code, Results & Conclusions

The following Python class sets up the grid and the matrix equation Eq. (4.10). Functions defined inside this class will be used in what follows.

```


import time
from numpy import zeros, size, sqrt, linspace
import scipy.linalg as la



```

[1] I chose to do the latter, since the code is written in Python anyway. For higher efficiency I would have used C++ instead, but due to time constraints I went with Python since it has more libraries “working out of the box” in the Anaconda distribution.

```
#==============================================================
#       CLASS THAT SETS UP GRID & MATRIX EQUATION
#==============================================================

class NonlinearPoisson3D:

    #Constructor/Initializer  (arguments are the Cartesian coordinates)
    def __init__(self, x, y, z):

        self.N = size(x)          #equal grid size on all dimensions x,y,z
        self.h = x[1] - x[0]      #equal grid spacing h = delta x = delta y = delta z

        self.b_1d = zeros(self.N ** 3)                    #initialize b long vector
        self.A = zeros((self.N ** 3, self.N ** 3))        #initialize matrix A
        self.sol = zeros((self.N, self.N, self.N))        #initialize solution
        self.rad = zeros((self.N, self.N, self.N))        #initialize radius


        #compute radius
        for i in range(0, self.N):
            for j in range(0, self.N):
                for k in range(0, self.N):
                    rad2 = (x[i] ** 2) + (y[j] ** 2) + (z[k] ** 2)
                    self.rad[i, j, k] = sqrt(rad2)


    def operator_matrix(self, f_prime):
        """Set up operator matrix A of coefficients (Eq. (4.10))"""

        N = self.N

        """Set Robin BCs (see Eq.(4.11) and the discussion that follows)"""
        i = 0  # lower x-boundary
        for j in range(0, N):
            for k in range(0, N):
                index = self.super_index(i, j, k)
                self.A[index, index] = self.rad[i, j, k]
                self.A[index, index + 1] = -self.rad[i + 1, j, k]

        i = N - 1  # upper x-boundary
        for j in range(0, N):
            for k in range(0, N):
                index = self.super_index(i, j, k)
                self.A[index, index] = self.rad[i, j, k]
                self.A[index, index - 1] = -self.rad[i - 1, j, k]

        j = 0  # lower y-boundary
        for i in range(1, N - 1):
            for k in range(0, N):
                index = self.super_index(i, j, k)
                self.A[index, index] = self.rad[i, j, k]
                self.A[index, index + N] = -self.rad[i, j + 1, k]

        j = N - 1  # upper y-boundary
        for i in range(1, N - 1):
            for k in range(0, N):
                index = self.super_index(i, j, k)
                self.A[index, index] = self.rad[i, j, k]
                self.A[index, index - N] = -self.rad[i, j - 1, k]

        k = 0  # lower z-boundary
        for i in range(1, N - 1):
            for j in range(1, N - 1):
                index = self.super_index(i, j, k)
                self.A[index, index] = self.rad[i, j, k]
                self.A[index, index + N**2] = -self.rad[i, j, k + 1]

        k = N - 1  # upper z-boundary
        for i in range(1, N - 1):
            for j in range(1, N - 1):
                index = self.super_index(i, j, k)
```

```
                self.A[index, index] = self.rad[i, j, k]
                self.A[index, index - N**2] = -self.rad[i, j, k - 1]

        """Use Eq. (4.10) to fill matrix A"""

        for i in range(1, N - 1):
            for j in range(1, N - 1):
                for k in range(1, N - 1):
                    index = self.super_index(i, j, k)

                    # diagonal elements (recall that G in Eq.(4.10) is - f')
                    self.A[index, index] = - (self.h ** 2) * f_prime[i, j, k] - 6.0

                    # off-diagonal elements
                    self.A[index, index - 1] = 1.0
                    self.A[index, index + 1] = 1.0
                    self.A[index, index - N] = 1.0
                    self.A[index, index + N] = 1.0
                    self.A[index, index - N**2] = 1.0
                    self.A[index, index + N**2] = 1.0


    def rhs(self, b):
        """Setup RHS of matrix equation (4.10)"""

        N = self.N
        for i in range(1, N - 1):
            for j in range(1, N - 1):
                for k in range(1, N - 1):
                    index = self.super_index(i, j, k)
                    self.b_1d[index] = (self.h ** 2) * b[i, j, k]


    def solve(self):

        #Find solution (in long vector (1d) format)
        sol_1d = la.solve(self.A, self.b_1d)

        #Now translate from superindex to 3d format
        for i in range(0, self.N):
            for j in range(0, self.N):
                for k in range(0, self.N):
                    index = self.super_index(i, j, k)
                    self.sol[i, j, k] = sol_1d[index]

        return self.sol     #solution in full 3d format


    def super_index(self, i, j, k):
        """This is the super index we've been using throughout (see Eq.(4.9))"""
        return i + (self.N * j) + ((self.N**2) * k)
```

Now that the solver is all set up, we are finally ready to construct our initial data. We note that in the code we modify the radial coordinate $r = \sqrt{x^2 + y^2 + z^2}$ that appears in the Bowen-York curvature (c.f., Eqs. (3.22)) as well as in the expression for ϑ (c.f., Eq. (3.27)), since we want the flexibility of setting coordinates for the location of the black hole that are not limited to the origin of the Cartesian grid. To that end, we define

$$r_{\mathrm{BH}} = \sqrt{(x - x_{\mathrm{BH}})^2 + (y - y_{\mathrm{BH}})^2 + (z - z_{\mathrm{BH}})^2}, \tag{4.12}$$

where $(x_{\mathrm{BH}}, y_{\mathrm{BH}}, z_{\mathrm{BH}})$ are coordinates that specify the black hole's location in the grid. The data we shall construct is for a single black hole, so that the function ϑ in Eq. (3.27) is simply

$$\vartheta = \frac{2r}{M}. \tag{4.13}$$

In fact, let us comment on the physical units. In the geometrized units we have been using throughout

($G = c = 1$), physical quantities such as mass and length share the same unit; whence we nondimensionalize our physical parameters by setting

$$\bar{x}^i = \frac{x^i}{M}, \qquad \bar{P}^i = \frac{P^i}{M}, \qquad \bar{J}^i = \frac{J^i}{M^2}. \tag{4.14}$$

These "barred" quantities are the ones we will be using in our code. Of course, we could have also set $M = 1$, but by using nondimensional units we avoid committing to a specific black hole mass M. We can easily do calculations for a given mass by multiplying the parameters in Eq. (4.14) by the correct factor of M.

The following class constructs all the terms needed to construct the initial data (i.e., the Bowen-York curvature, the linear and angular momenta, the functions ϑ and ϱ, etc). We use functions from the previously defined `NonlinearPoisson3D` class.

```
#==========================================================================
#    CLASS THAT CONSTRUCTS PUNCTURE INITIAL DATA FOR A SINGLE BLACK HOLE
#==========================================================================

class InitialData:

    def __init__(self, bh_loc, ang_mom, lin_mom, N, bd):
        """Constructor/Initializer  (arguments are physical parameters,
           number of gridpoints, and outer boundary)"""

        self.bh_loc = bh_loc          #location of black hole
        self.ang_mom = ang_mom        #angular momentum of black hole
        self.lin_mom = lin_mom        #linear momentum of black hole

        #Set up the grid
        self.N = N                    #number of gridpoints
        self.bd = bd                  #outer boundary
        self.h = (2.0 * bd)/N         #h = ( bd - (-bd) )/N

        #Set up the coordinates using cell-centered grid
        half_h = self.h/2.0
        self.x = linspace(half_h - bd, bd -
                          half_h, N)
        self.y = linspace(half_h - bd, bd -
                          half_h, N)
        self.z = linspace(half_h - bd, bd -
                          half_h, N)

        #Allocate the elliptic solver using the NonlinearPoisson3D class
        self.solver = NonlinearPoisson3D(self.x, self.y, self.z)

        #Initialize functions u, theta, rho, and residual R (here we call it res)
        self.theta = zeros((N, N, N))
        self.rho = zeros((N, N, N))
        self.u = zeros((N, N, N))
        self.res = zeros((N, N, N))


    def solution(self, tol, it_max):
        """Construct the solution within a user-set tolerance
           and max number of iterations allowed"""

        #theta_rho_functs and residual will be defined shortly
        self.theta_rho_functs()
        res_norm = self.residual()

        #Iterate
        it_step = 0
        while res_norm > tol and it_step < it_max:
            it_step += 1
            self.update_u()               #update_u also to be defined shortly
            res_norm = self.residual()
            print(" Residual after", it_step, "iterations :", res_norm)
        if (res_norm < tol):
```

```
            print(" Done. Reached convergence within desired tolerance!")
        else:
            print(" No convergence, unfortunately :( )")


    def update_u(self):
        """Function that implements one iteration: u^{[n+1]} = u^{[n]} + \delta u"""

        N = self.N
        f_prime = zeros((N, N, N))     #initialize f'
        b = zeros((N, N, N))           #initialize b  (=-R)

        for i in range(1, N - 1):
            for j in range(1, N - 1):
                for k in range(1, N - 1):
                    #calculate f' from Eq.(4.6)
                    var_exp = self.theta[i, j, k] * (1.0 + self.u[i, j, k]) + 1.0
                    f_prime[i, j, k] = (7.0 * self.rho[i, j, k] *
                                    self.theta[i,j,k])/var_exp**8
                    #Set b=-R (-residual)
                    b[i, j, k] = -self.res[i, j, k]

        #Update the solver feeding it the newly calculated f'
        self.solver.operator_matrix(f_prime)

        #Also update using the newly calculated residual
        self.solver.rhs(b)

        #Solve for \delta u (recall Eq.(4.5))
        delta_u = self.solver.solve()

        #Update u (u^{[n+1]} = u^{[n]} + delta u)
        self.u += delta_u


    def residual(self):
        """Calculate the residual from Eq.(4.2) using updated u values"""

        res_norm = 0.0
        for i in range(1, self.N - 1):
            for j in range(1, self.N - 1):
                for k in range(1, self.N - 1):

                    """Compute the Laplace operator \partial^2
                       (using 2nd order centered difference)"""
                    ddx = (self.u[i + 1, j, k] - 2.0 * self.u[i, j, k] +
                           self.u[i - 1, j, k])
                    ddy = (self.u[i, j + 1, k] - 2.0 * self.u[i, j, k] +
                           self.u[i, j - 1, k])
                    ddz = (self.u[i, j, k + 1] - 2.0 * self.u[i, j, k] +
                           self.u[i, j, k - 1])
                    laplace = (ddx + ddy + ddz)/(self.h ** 2)

                    #Now compute f(u)=  - rho/( theta*(1 + u) + 1)^7
                    f_in = self.theta[i, j, k] * (1.0 + self.u[i, j, k]) + 1.0 #expression inside parentheses in f
                    f = - self.rho[i, j, k]/(f_in ** 7)

                    self.res[i, j, k] = laplace - f        #R = laplace - f (recall Eq.(4.2))
                    res_norm += self.res[i, j, k] ** 2     #sum the square of all residuals

        res_norm = sqrt(res_norm) * (self.h ** 3)          #2 grid-norm of residual
        return res_norm


    def theta_rho_functs(self):
        """Set up functions theta and rho (see Eqs.(3.27) and (3.28), respectively)"""
        """Here we also compute the Bowen-York curvature, which is needed for rho"""

        N = self.N

```

```
        #define momenta
        j_x = self.ang_mom[0]
        j_y = self.ang_mom[1]
        j_z = self.ang_mom[2]

        p_x = self.lin_mom[0]
        p_y = self.lin_mom[1]
        p_z = self.lin_mom[2]

        for i in range(0, N):
            for j in range(0, N):
                for k in range(0, N):

                    #define radial function r_BH (see Eq.(4.12))
                    d_x = self.x[i] - self.bh_loc[0]
                    d_y = self.y[j] - self.bh_loc[1]
                    d_z = self.z[k] - self.bh_loc[2]
                    r_bh = sqrt( (d_x ** 2) + (d_y ** 2) + (d_z ** 2))

                    #recall l^i radial unit vector from Eqs. (3.21)
                    l_x = d_x/r_bh
                    l_y = d_y/r_bh
                    l_z = d_z/r_bh

                    #Construct Bowen-York curvature with ang mom A_J^{ij} (Eq. (3.22a))
                    J_coeff = 3.0/(r_bh**3)
                    Aj_xx = J_coeff * (2.0 * l_x * (j_y * l_z - j_z * l_y))
                    Aj_yy = J_coeff * (2.0 * l_y * (j_z * l_x - j_x * l_z))
                    Aj_zz = J_coeff * (2.0 * l_z * (j_x * l_y - j_y * l_x))
                    Aj_xy = J_coeff
                            *(l_x * (j_z * l_x - j_x * l_z) + l_y * (j_y * l_z - j_z * l_y))
                    Aj_xz = J_coeff
                            *(l_x * (j_x * l_y - j_y * l_x) + l_z * (j_y * l_z - j_z * l_y))
                    Aj_yz = J_coeff
                            *(l_y * (j_x * l_y - j_y * l_x) + l_z * (j_z * l_x - j_x * l_z))

                    #Construct Bowen-York curvature with lin mom A_p^{ij} (Eq. (3.22b))
                    P_coeff = 3.0/(2.0 * (r_bh**2))
                    lP = (l_x * p_x) + (l_y * p_y) + (l_z * p_z)     #contraction l_k P^k
                    Ap_xx = P_coeff * (2.0 * p_x * l_x + lP * (l_x * l_x - 1.0))
                    Ap_yy = P_coeff * (2.0 * p_y * l_y + lP * (l_y * l_y - 1.0))
                    Ap_zz = P_coeff * (2.0 * p_z * l_z + lP * (l_z * l_z - 1.0))
                    Ap_xy = P_coeff * (p_x * l_y + p_y * l_x + lP * l_x * l_y)
                    Ap_xz = P_coeff * (p_x * l_z + p_z * l_x + lP * l_x * l_z)
                    Ap_yz = P_coeff * (p_y * l_z + p_z * l_y + lP * l_y * l_z)

                    #Construct full Bowen-York curvature (Eq. (3.22c), with + sign)
                    A_xx = Ap_xx + Aj_xx
                    A_yy = Ap_yy + Aj_yy
                    A_zz = Ap_zz + Aj_zz
                    A_xy = Ap_xy + Aj_xy
                    A_xz = Ap_xz + Aj_xz
                    A_yz = Ap_yz + Aj_yz

                    #Compute A_{ij} A^{ij} term in rho (Eq.(3.28))
                    A2 = (
                          A_xx ** 2 + A_yy ** 2 + A_zz ** 2 +
                          2.0*(A_xy ** 2 + A_xz ** 2 + A_yz ** 2)
                         )

                    #Compute theta (Eq.(4.13)) and rho (Eq.(3.28))
                    self.theta[i, j, k] = 2.0 * r_bh
                    self.rho[i, j, k] = ( (self.theta[i, j, k] ** 7)/8.0 ) * A2


    def write_to_file(self):
        """Write solution to file"""

        filename = "InitialData_" + str(self.N) + "_" + str(self.bd)
        filename = filename + ".data"
        out = open(filename, "w")
```

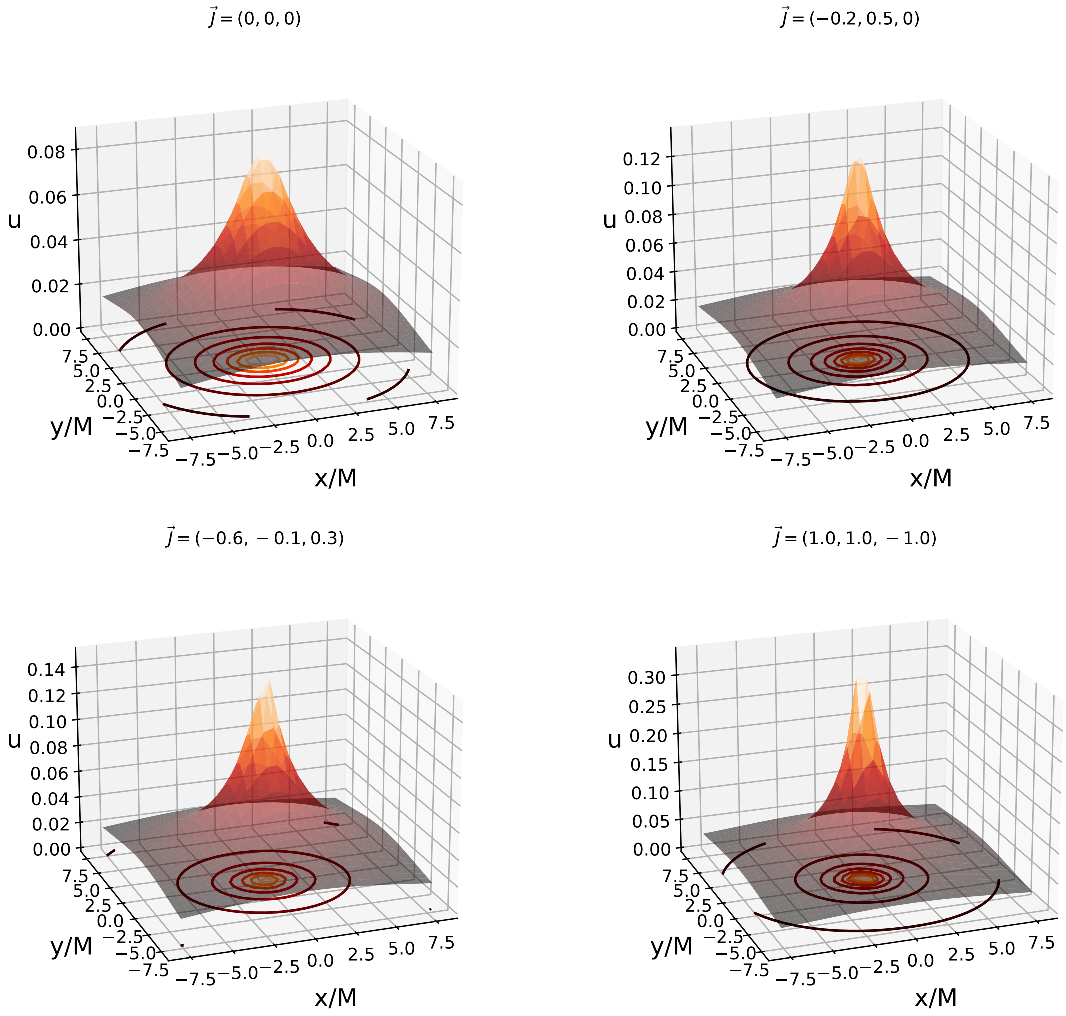
```
        if out:
            k = self.N // 2
            out.write(
                "# Data for black hole at x = (%f,%f,%f)\n"
                % (self.bh_loc[0], self.bh_loc[1], self.bh_loc[2])
            )
            out.write("# with angular momentum P = (%f, %f, %f)\n" %
                          (self.ang_mom))
            out.write("# and linear momentum P = (%f, %f, %f)\n" %
                          (self.lin_mom))
            out.write("# in plane for z = %e \n" % (self.z[k]))
            out.write("# x              y              u              \n")
            out.write("#=============================================\n")
            for i in range(0, self.N):
                for j in range(0, self.N):
                    out.write("%e  %e  %e\n" % (self.x[i], self.y[j],
                                                 self.u[i, j, k]))
                out.write("\n")
            out.close()
        else:
            print(" Could not open file ", filename," in write_to_file() function")
```

All the work has been done. Now we choose whatever parameters we want to impose on our black hole and build the solution. For example, say we want a black hole centered at the origin $(x_{\text{BH}}, y_{\text{BH}}, z_{\text{BH}}) = (0, 0, 0)$, with linear momentum $\vec{P} = (1, 0, 0)$ and angular momentum $\vec{J} = (-0.2, 0.5, 0)$ (both momenta must have entries with absolute value less than 1, due to the scaling (4.14)). Then we use the following routine to build this black hole and write the resulting object to a data file:

```
#=====================================================================
#                MAIN ROUTINE
#=====================================================================

def main():

    """Set default values for variables:"""

    #location of black hole:
    loc_x = 0.0
    loc_y = 0.0
    loc_z = 0.0

    #linear momentum entries:
    p_x = 1.0
    p_y = 0.0
    p_z = 0.0

    #angular momentum entries:
    j_x = -0.2
    j_y = 0.5
    j_z = 0.0

    N = 26            #number of grid points
    bd = 8.0          #location of outer boundary
    tol = 1.0e-12     #tolerance
    it_max = 50       #max number of iterations allowed

    bh_loc = ( loc_x, loc_y, loc_z )    #location of black hole
    lin_mom = ( p_x, p_y, p_z )         #linear momentum
    ang_mom = ( j_x, j_y, j_z )         #angular momentum

    #Construct the initial data solver
    bh_initdata = InitialData(bh_loc, ang_mom, lin_mom, N, bd)

    #Build solution
    bh_initdata.solution(tol, it_max)

    #Output to file
    bh_initdata.write_to_file()
```

```python

if __name__ == '__main__':
    start_time = time.time()
    main()
    print("It took %s seconds to run this beautiful code :)" % (time.time() - start_time))
```

Since our main interest in this investigation is the spin of the black hole, we run this routine for several values of $\vec{J}$ (fixing $(x_{\mathrm{BH}}, y_{\mathrm{BH}}, z_{\mathrm{BH}}) = (0,0,0)$ and $\vec{P} = (1,0,0)$) and report the results in the following figures. We supress one spatial dimension by setting $z = 0$, and include contour lines for u at the $u = 0$ plane. A very coarse grid ($N = 26$) is used; if we refine further we are likely to run out of memory allocation (in hindsight, sparse allocation could have been a good workaround). Nevertheless, the code was run for even coarser grids ($N \in \{16, 18, 20, 22, 24\}$), and all cases show the same irregular behavior for u at the puncture when we increase the spin. Note that we are plotting the correction term u and not the full solution ψ, but plotting the latter does not change anything meaningful in the results since it is merely a translation in space: $\psi = 1 + 1/(2r) + u$ (c.f., Eq. (3.27)).



As we can see from the figures, as the spin of the black hole increases, the function u becomes ever less smooth at the puncture $(x_{\mathrm{BH}}, y_{\mathrm{BH}}, z_{\mathrm{BH}}) = (0,0,0)$. The code never fails to converge (u never blows up), even for the maximal spin case shown in the bottom right figure, but nevertheless we do find this odd irregular behavior of u that gets worse as the spin increases. This may perhaps be a sign of the limitations of the Bowen-York data? It is known that a rotating (Kerr) black hole does not admit a conformally-flat spatial geometry, and the latter is a crucial assumption in the Bowen-York model. In practice, if we prescribe Bowen-York data with very high spin to a binary black hole system, we find that the black holes quickly lose some of this spin and settle for more mild angular momenta. The resulting loss of energy appears as some spurious gravitational wave signal, which is typically ignored since we know that it is simply not natural (we expect gravitational waves to appear in the final orbits and plunge of the inspiral, not at the very beginning of the simulation when the black holes are too far apart). This inability of the Bowen-York data to cope with very high spins is thought to be due to the aforementioned incompatibility of rotating black holes and flat spatial geometries. I believe that the irregularity for the correction term u for high spins that we have shown in this report may be providing some "under the hood" peek at the limitations of the Bowen-York model. Further investigation will involve evolving this data in time and monitoring constraint violation as well as the behavior of the extrinsic curvature.

A

Proof of Gauss-Codazzi, Codazzi-Mainardi, & Ricci Equations

In this appendix we will write out detailed calculations that prove the Gauss-Codazzi, Codazzi-Mainardi, and Ricci Equations, all three of which we use in the main text to derive projections of the ambient (4D) spacetime curvature onto the (3D) spacelike hypersurfaces.

A.1. Proof of Gauss-Codazzi

Recall that he Riemann tensor is defined in terms of second covariant derivatives of a vector (Ricci identity),

$$2\nabla_{[c}\nabla_{d]}V^a = {}^{(4)}R^a{}_{bcd}V^b. \tag{A.1}$$

Thus, to relate ${}^{(4)}R^a{}_{bcd}$ to $R^a{}_{bcd}$, it is natural to consider the Ricci identity for the projected spatial derivative. We start there:

$$\begin{aligned} D_a D_b V^c = D_a\left(D_b V^c\right) &= \gamma_a{}^d\gamma_b{}^e\gamma^c{}_f\,\nabla_d(D_e V^f) \\ &= \gamma_a{}^d\gamma_b{}^e\gamma^c{}_f\,\nabla_d\left(\gamma_e{}^g\gamma^f{}_h\nabla_g V^h\right). \end{aligned} \tag{A.2}$$

In order to expand this further, we will make use of these facts:

$$\begin{aligned} \nabla_d\gamma_e{}^g &= \nabla_d\left(\delta_e{}^g + n_e n^g\right) = \nabla_d(n_e n^g) = n_e\nabla_d n^g + n^g\nabla_d n_e; \\ \gamma_b{}^e n_e &= 0; \\ n_a V^a &= 0 \implies n_a\nabla_b V^a = -V^a\nabla_b n_a; \\ \gamma^a{}_b\gamma^b{}_c &= \gamma^a{}_c; \\ 0 &= \nabla_d\left(\gamma^c{}_f n^f\right) = \gamma^c{}_f\nabla_d n^f + n^f\nabla_d(n^c n_f) = \gamma^c{}_f\nabla_d n^f - \nabla_d n^c \\ &\implies \gamma^c{}_f\nabla_d n^f = \nabla_d n^c. \end{aligned}$$

Now we may expand (A.2):

$$\begin{aligned} D_a D_b V^c &= \gamma_a{}^d\gamma_b{}^e\gamma^c{}_f\,\nabla_d\left(\gamma_e{}^g\gamma^f{}_h\nabla_g V^h\right) \\ &= \gamma_a{}^d\gamma_b{}^e\gamma^c{}_f\left\{\gamma^f{}_h\nabla_g V^h\nabla_d\gamma_e{}^g + \gamma_e{}^g\nabla_g V^h\nabla_d\gamma^f{}_h + \gamma_e{}^g\gamma^f{}_h\nabla_d\nabla_g V^h\right\} \\ &= \gamma_a{}^d\gamma_b{}^e\gamma^c{}_f\{\gamma^f{}_h\nabla_g V^h\left(n_e\nabla_d n^g + n^g\nabla_d n_e\right) \\ &\quad + \gamma_e{}^g\nabla_g V^h(n_h\nabla_d n^f + n^f\nabla_d n_h) + \gamma_e{}^g\gamma^f{}_h\nabla_d\nabla_g V^h\} \end{aligned}$$

$$
\begin{aligned}
&= \gamma_a{}^d \gamma_b{}^e \gamma^c{}_f \{\gamma^f{}_h \nabla_g V^h n^g \nabla_d n_e + \gamma_e{}^g \nabla_g V^h n_h \nabla_d n^f \\
&\quad + \gamma_e{}^g \gamma^f{}_h \nabla_d \nabla_g V^h\} \qquad \text{(Since } \gamma_b{}^a n_a = 0) \\
&= \gamma_a{}^d \gamma_b{}^e \underbrace{\gamma^c{}_f \gamma^f{}_h}_{=\gamma^c{}_h} n^g \nabla_g V^h \nabla_d n_e + \gamma_a{}^d \underbrace{\gamma_b{}^e \gamma_e{}^g}_{=\gamma_b{}^g} \gamma^c{}_f \nabla_d n^f \underbrace{n_h \nabla_g V^h}_{=-V^h \nabla_g n_h} \\
&\quad + \gamma_a{}^d \underbrace{\gamma_b{}^e \gamma_e{}^g}_{=\gamma_b{}^g} \underbrace{\gamma^c{}_f \gamma^f{}_h}_{=\gamma^c{}_h} \nabla_d \nabla_g V^h \\
&= \underbrace{\gamma_a{}^d \gamma_b{}^e \nabla_d n_e}_{=-K_{ab}} \gamma^c{}_h n^g \nabla_g V^h - \gamma_a{}^d \gamma_b{}^g \gamma^c{}_f \nabla_d n^f \underbrace{\nabla_g n_h}_{=\gamma_h{}^p \nabla_g n_p} V^h + \gamma_a{}^d \gamma_b{}^g \gamma^c{}_h \nabla_d \nabla_g V^h \\
&= -K_{ab} \gamma^c{}_h n^g \nabla_g V^h - \underbrace{\gamma_a{}^d \gamma^c{}_f \nabla_d n^f}_{=-K_a{}^c} \underbrace{\gamma_b{}^g \gamma_h{}^p \nabla_g n_p}_{=-K_{bh}} V^h + \gamma_a{}^d \gamma_b{}^g \gamma^c{}_h \nabla_d \nabla_g V^h \\
&= -K_{ab} \gamma^c{}_h n^g \nabla_g V^h - K_a{}^c K_{bh} V^h + \gamma_a{}^d \gamma_b{}^g \gamma^c{}_h \nabla_d \nabla_g V^h.
\end{aligned}
$$

Permuting the indices a and b and substracting from the above result to form $D_a D_b V^c - D_b D_a V^c$, the first term vanishes since K_{ab} is symmetric, and so we are left with

$$
D_a D_b V^c - D_b D_a V^c = \left(K_b{}^c K_{ah} - K_a{}^c K_{bh}\right) V^h + \gamma_a{}^d \gamma_b{}^g \gamma^c{}_h \left(\nabla_d \nabla_g V^h - \nabla_g \nabla_d V^h\right). \tag{A.3}
$$

Now, applying both the 3D and 4D Ricci identities to (A.3), we get

$$
R^c{}_{fab} V^f = \left(K_b{}^c K_{af} - K_a{}^c K_{bf}\right) V^f + \gamma_a{}^d \gamma_b{}^g \gamma^c{}_h \, {}^{(4)}R^h_{fdg} V^f,
$$

or equivalently, since $V^f = \gamma^f{}_p V^p$,

$$
\gamma_a{}^d \gamma_b{}^g \gamma^c{}_h \gamma_p{}^f \, {}^{(4)}R^h_{fdg} V^p = R^c{}_{pab} V^p + \left(K_a{}^c K_{bp} - K_b{}^c K_{ap}\right) V^p.
$$

But this relation must hold for any spatial vector V^p, so we have proven (1.43a):

$$
\boxed{\gamma_a{}^e \gamma_b{}^f \gamma^g{}_c \gamma_d{}^h \, {}^{(4)}R^c_{hef} = R^g{}_{dab} + K_a{}^g K_{bd} - K_b{}^g K_{ad}} \tag{A.4}
$$

Equivalently, hitting (A.4) with g_{cg} on both sides,

$$
\begin{aligned}
\gamma_a{}^e \gamma_b{}^f \gamma^g{}_c \gamma_d{}^h \, {}^{(4)}R^c_{hef} \, g_{cg} &= g_{cg} R^g{}_{dab} + g_{cg} K_a{}^g K_{bd} - g_{cg} K_b{}^g K_{ad} \\
\gamma_a{}^e \gamma_b{}^f \gamma^g{}_c \gamma_d{}^h \, {}^{(4)}R_{ghef} &= \gamma_{cg} R^g{}_{dab} + \gamma_{cg} K_a{}^g K_{bd} - \gamma_{cg} K_b{}^g K_{ad}
\end{aligned}
$$

$$
\boxed{\gamma_a{}^e \gamma_b{}^f \gamma_c{}^g \gamma_d{}^h \, {}^{(4)}R_{efgh} = R_{abcd} + K_{ac} K_{bd} - K_{ad} K_{cb}} \tag{A.5}
$$

A.2. Proof of Codazzi-Mainardi

First consider the spatial derivative of the extrinsic curvature:

$$
\begin{aligned}
D_a K_{bc} = \gamma_a{}^d \gamma_b{}^e \gamma_c{}^f \nabla_d K_{ef} &= \gamma_a{}^d \gamma_b{}^e \gamma_c{}^f \nabla_d \left(-\gamma_e{}^g \gamma_f{}^h \nabla_g n_h\right) \\
&= -\gamma_a{}^d \gamma_b{}^e \gamma_c{}^f \left(\nabla_d \nabla_e n_f + \nabla_d (n_e \mathsf{a}_f)\right) \\
&= -\gamma_a{}^d \gamma_b{}^e \gamma_c{}^f \nabla_d \nabla_e n_f - \gamma_a{}^d \gamma_c{}^f \underbrace{\gamma_b{}^e n_e}_{=0} \nabla_d \mathsf{a}_f - \underbrace{\gamma_c{}^f \mathsf{a}_f}_{=\mathsf{a}_c} \underbrace{\gamma_a{}^d \gamma_b{}^e \nabla_d n_e}_{=-K_{ab}}
\end{aligned}
$$

$$= -\gamma_a{}^d \gamma_b{}^e \gamma_c{}^f \nabla_d \nabla_e n_f + \mathsf{a}_c K_{ab}.$$

Now, since K_{ab} is symmetric, the last term disappears when antisymmetrizing, and we are left with

$$D_{[a} K_{b]} c = -\gamma_a{}^d \gamma_b{}^e \gamma_c{}^f \nabla_{[d} \nabla_{e]} n_f. \tag{A.6}$$

Using the Ricci identity, we get

$$\begin{aligned} 2\nabla_{[d}\nabla_{e]} n_f &= (\nabla_d \nabla_e - \nabla_e \nabla_d) n_f \\ &= -{}^{(4)}R^h{}_{fde} n_h = -n^p g_{hp} {}^{(4)}R^h{}_{fde} \\ &= -n^p \, {}^{(4)}R_{pfde}. \end{aligned}$$

Applying this to the RHS of (A.6), we get

$$D_{[a} K_{b]} c = \gamma_a{}^d \gamma_b{}^e \gamma_c{}^f n^p \, {}^{(4)}R_{pfde},$$

or similarly, applying the symmetries

$${}^{(4)}R_{pfde} = {}^{(4)}R_{depf} \quad \text{and} \quad {}^{(4)}R_{depf} = -{}^{(4)}R_{defp}$$

we arrive at (1.43b):

$$\boxed{D_b K_{ac} - D_a K_{bc} = \gamma_a{}^d \gamma_b{}^e \gamma_c{}^f n^p \, {}^{(4)}R_{defp}} \tag{A.7}$$

Thanks to the symmetries of the Riemann tensor, changing the index contracted with n^p would not give an independent relation; it would at most result in a change of sign of the right-hand side.

A.3. Proof of Ricci Equation

In the proof we will use the previous results (1.32) and (1.33)

$$\mathsf{a}_a = D_a \log \alpha \qquad \text{and} \qquad D_a \mathsf{a}_b = \frac{1}{\alpha} D_a D_b \alpha - \mathsf{a}_a \mathsf{a}_b,$$

as well as the facts

$$\begin{aligned} K_{ab} = -\nabla_a n_b - n_a \mathsf{a}_b \;&\Longrightarrow\; \nabla_a n_b = -K_{ab} - n_a \mathsf{a}_b; \\ {}^{(4)}R^e{}_{bac} n_e = 2\nabla_{[c}\nabla_{a]} n_b \quad &\& \quad {}^{(4)}R^e{}_{bac} = g^{de}\,{}^{(4)}R_{dbac} \\ &\Longrightarrow\; {}^{(4)}R_{dbac} n^d = 2\nabla_{[c}\nabla_{a]} n_b. \end{aligned}$$

Let us compute the Lie derivative of K_{ab} in the direction of the normal n^a:

$$\begin{aligned} \mathcal{L}_{\vec{n}} K_{ab} &= n^c \nabla_c K_{ab} + K_{cb} \nabla_a n^c + K_{ac} \nabla_b n^c \\ &= n^c \nabla_c (-\nabla_a n_b - n_a \mathsf{a}_b) + K_{cb}(-K_a{}^c - n_a \mathsf{a}^c) + \underbrace{K_{ac}}_{=K_{ca}} (-K_b{}^c - n_b \mathsf{a}^c) \\ &= -n^c \nabla_c \nabla_a n_b - n^c \nabla_c (n_a \mathsf{a}_b) - K_{cb} K_a{}^c - K_{ca} K_b{}^c - K_{cb} n_a \mathsf{a}^c - K_{ca} n_b \mathsf{a}^c \\ &= \underbrace{-n^c \nabla_c \nabla_a n_b}_{=-{}^{(4)}R_{dbac} n^d n^c - n^c \nabla_a \nabla_c n_b} \; -n_a n^c \nabla_c \mathsf{a}_b - \mathsf{a}_b \underbrace{n^c \nabla_c n_a}_{=\mathsf{a}_a} - K_{cb} K_a{}^c - K_{ca} K_b{}^c \\ &\quad - K_{cb} n_a \mathsf{a}^c - K_{ca} n_b \mathsf{a}^c \\ &= -n^c n^d \, {}^{(4)}R_{dbac} - n^c \nabla_a \nabla_c n_b - n_a n^c \nabla_c \mathsf{a}_b - \mathsf{a}_b \mathsf{a}_a - 2K_{c(b} K_{a)}{}^c - 2K_{c(b} n_{a)} \mathsf{a}^c. \end{aligned}$$

Expanding upon the second term above,

$$\nabla_a \underbrace{(n^c \nabla_c n_b)}_{=\mathsf{a}_b} = n^c \nabla_a \nabla_c n_b + \nabla_c n_b \nabla_a n^c$$

$$
\begin{aligned}
\implies n^c\nabla_a\nabla_c n_b &= \nabla_a \mathrm{a}_b - \nabla_c n_b\,\nabla_a n^c\\
&= \nabla_a \mathrm{a}_b - (-K_{cb} - n_c\mathrm{a}_b)(-K_a{}^c - n_a\mathrm{a}^c)\\
&= \nabla_a \mathrm{a}_b - (K_{cb}K_a{}^c + K_{cb}n_a\mathrm{a}^c + \mathrm{a}_b\underbrace{n_cK_a{}^c}_{=0} + \mathrm{a}_b n_a\underbrace{n_c\mathrm{a}^c}_{=0})\\
&= \nabla_a \mathrm{a}_b - K_{cb}K_a{}^c - K_{cb}n_a\mathrm{a}^c.
\end{aligned}
$$

Thus, we have

$$
\begin{aligned}
\mathcal{L}_{\vec{n}}K_{ab} &= -n^cn^d\,{}^{(4)}R_{dbac} - n^c\nabla_a\nabla_c n_b - n_an^c\nabla_c\mathrm{a}_b - \mathrm{a}_b\mathrm{a}_a - 2K_{c(b}K_{a)}{}^c - 2K_{c(b}n_{a)}\mathrm{a}^c\\
&= -n^cn^d\,{}^{(4)}R_{dbac} - (\nabla_a\mathrm{a}_b - K_{cb}K_a{}^c - K_{cb}n_a\mathrm{a}^c) - n_an^c\nabla_c\mathrm{a}_b - \mathrm{a}_b\mathrm{a}_a\\
&\quad - K_{cb}K_a{}^c - K_{ca}K_b{}^c - K_{cb}n_a\mathrm{a}^c - K_{ca}n_b\mathrm{a}^c\\
&= -n^cn^d\,{}^{(4)}R_{dbac} - \nabla_a\mathrm{a}_b - n_an^c\nabla_c\mathrm{a}_b - \mathrm{a}_b\mathrm{a}_a - K_{ca}K_b{}^c - K_{ca}n_b\mathrm{a}^c.
\end{aligned}
$$

Now, using

$$
\begin{aligned}
n^a\nabla_a\underbrace{(K_{cb}n^c)}_{=0} &= n^an^c\nabla_aK_{cb} + K_{cb}n^a\nabla_an^c\\
\implies K_{cb}n^a\nabla_an^c &= -n^an^c\nabla_aK_{cb}\\
&= -n^cn^a\nabla_cK_{ab}, \qquad\qquad \text{(relabeling } a\leftrightarrow c)
\end{aligned}
$$

we can show that $\mathcal{L}_{\vec{n}}K_{ab}$ is purely spatial, i.e.,

$$
\begin{aligned}
n^a\mathcal{L}_{\vec{n}}K_{ab} &= n^an^c\nabla_cK_{ab} + K_{cb}n^a\nabla_an^c + \underbrace{n^aK_{ac}}_{=0}\nabla_bn^c\\
&= n^an^c\nabla_cK_{ab} - n^cn^a\nabla_cK_{ab}\\
&= 0.
\end{aligned}
$$

Thus, projecting onto the hypersurface the result

$$
\mathcal{L}_{\vec{n}}K_{ab} = -n^cn^d\,{}^{(4)}R_{dbac} - \nabla_a\mathrm{a}_b - n_an^c\nabla_c\mathrm{a}_b - \mathrm{a}_b\mathrm{a}_a - K_{ca}K_b{}^c - K_{ca}n_b\mathrm{a}^c \tag{A.8}
$$

does not affect the left hand side, given that $\mathcal{L}_{\vec{n}}K_{ab}$ is purely spatial. Hence, since we have two free indices (a, b) on (A.8), we apply the projection operator twice:

$$
\begin{aligned}
\mathcal{L}_{\vec{n}}K_{ab} &= \gamma_a{}^e\gamma_b{}^f\mathcal{L}_{\vec{n}}K_{ef}\\
&= -n^cn^d\gamma_a{}^e\gamma_b{}^f\underbrace{{}^{(4)}R_{dfec}}_{=-{}^{(4)}R_{dfce}} - \underbrace{\gamma_a{}^e\gamma_b{}^f\nabla_e\mathrm{a}_f}_{=D_a\mathrm{a}_b} - \gamma_b{}^f\underbrace{\gamma_a{}^en_e}_{=0}n^c\nabla_c\mathrm{a}_f\\
&\quad - \gamma_a{}^e\gamma_b{}^f\underbrace{\mathrm{a}_e\mathrm{a}_f}_{\text{purely spatial}} - \gamma_a{}^e\gamma_b{}^f\underbrace{K_{ce}K_f{}^c}_{\text{purely spatial}} - \gamma_a{}^e\underbrace{\gamma_b{}^fn_f}_{=0}K_{ce}\mathrm{a}^c\\
&= n^cn^d\gamma_a{}^e\gamma_b{}^f\,{}^{(4)}R_{dfce} - \underbrace{D_a\mathrm{a}_b}_{=\frac{1}{\alpha}D_aD_b\alpha - \mathrm{a}_a\mathrm{a}_b} - \mathrm{a}_a\mathrm{a}_b - K_{ca}K_b{}^c\\
&= n^cn^d\gamma_a{}^e\gamma_b{}^f\,{}^{(4)}R_{dfce} - \frac{1}{\alpha}D_aD_b\alpha - K_{ac}K_b{}^c.
\end{aligned}
$$

This concludes our proof of (1.43c),

$$
\boxed{\gamma_a{}^e\gamma_b{}^fn^cn^d\,{}^{(4)}R_{ecfd} = \mathcal{L}_{\vec{n}}K_{ab} + \frac{1}{\alpha}D_aD_b\alpha + K_b{}^cK_{ac}} \tag{A.9}
$$

B

Weyl Transformations

One of the key steps in the BSSN formulation of 3+1 numerical relativity is the decomposition of the spatial Ricci tensor and Ricci scalar into their conformal relatives and additional terms that follow due to the rescaling of the metric. We show these derivations in gory detail here in the appendix, since its inclusion in the main text would have been an unwanted tangent.

First off we want to know how D and $\bar{D}$ are related; therefore a good starting point for our discussion would be to examine the relation between different connections on a manifold. [1] We start by considering the relation between the covariant derivative ∇_a of a connection ∇ and the covariant derivative $\widehat{\nabla}_a$ of a connection $\widehat{\nabla}$. Applying these covariant derivatives to some $\binom{a}{b}$ tensor field $\boldsymbol{T}$, we have

$$\nabla_c T^{i_1 \dots i_a}{}_{j_1 \dots j_b} = \widehat{\nabla}_c T^{i_1 \dots i_a}{}_{j_1 \dots j_b} + \sum_{d=1}^{a} T^{i_1 \dots e \dots i_a}{}_{j_1 \dots j_b}\, \mathfrak{C}^{i_d}{}_{ec} - \sum_{d=1}^{b} T^{i_1 \dots i_a}{}_{j_1 \dots e \dots j_b}\, \mathfrak{C}^{e}{}_{j_d c}, \tag{B.1}$$

where $\mathfrak{C}^c{}_{ab}$ is a symmetric ($\mathfrak{C}^c{}_{ab} = \mathfrak{C}^c{}_{ba}$) $\binom{1}{2}$ tensor field that encodes information regarding possible disagreements between the two connections ∇ and $\widehat{\nabla}$. We shall derive an expression for $\mathfrak{C}^c{}_{ab}$ straight away.

Applying (B.1) to the metric g_{ab} that is compatible with the connection ∇, we get

$$\begin{aligned} \underbrace{\nabla_c g_{ab}}_{=0} &= \widehat{\nabla}_c g_{ab} - \mathfrak{C}^d{}_{ac}\, g_{bd} - \mathfrak{C}^d{}_{bc}\, g_{ad}, \\ \implies \widehat{\nabla}_c g_{ab} &= \mathfrak{C}^d{}_{ac}\, g_{bd} + \mathfrak{C}^d{}_{bc}\, g_{ad} = \mathfrak{C}_{bac} + \mathfrak{C}_{abc}. \end{aligned} \tag{B.2}$$

Similarly, cyclic permutations yield

$$\widehat{\nabla}_a g_{cb} = \mathfrak{C}_{bca} + \mathfrak{C}_{cba} \tag{B.3}$$

$$\widehat{\nabla}_b g_{ac} = \mathfrak{C}_{acb} + \mathfrak{C}_{cab}. \tag{B.4}$$

Now we add (B.2) and (B.3) and subtract (B.4),

$$\begin{aligned} \widehat{\nabla}_c g_{ab} + \widehat{\nabla}_a g_{cb} - \widehat{\nabla}_b g_{ac} &= \mathfrak{C}_{bac} + \mathfrak{C}_{abc} + \underbrace{\mathfrak{C}_{bca}}_{=\mathfrak{C}_{bac}} + \mathfrak{C}_{cba} - \underbrace{\mathfrak{C}_{acb}}_{=\mathfrak{C}_{abc}} - \underbrace{\mathfrak{C}_{cab}}_{=\mathfrak{C}_{cba}} \\ &= 2\,\mathfrak{C}_{bac} \\ \implies \mathfrak{C}_{bac} &= \frac{1}{2}\left(\widehat{\nabla}_c g_{ab} + \widehat{\nabla}_a g_{cb} - \widehat{\nabla}_b g_{ac}\right) \end{aligned}$$

[1] For more detail, the reader may consult, e.g. [26].

$$\implies \mathfrak{C}^d{}_{ac} = \frac{1}{2} g^{db} \left(\widehat{\nabla}_c g_{ab} + \widehat{\nabla}_a g_{cb} - \widehat{\nabla}_b g_{ac} \right).$$

Thus we have found an expression for $\mathfrak{C}^c{}_{ab}$, relating a metric g_{ab} to the connection $\widehat{\nabla}$ of another metric $\widehat{g}_{ab}$,

$$\boxed{\mathfrak{C}^c{}_{ab} = \frac{1}{2} g^{cd} \left(\widehat{\nabla}_a g_{bd} + \widehat{\nabla}_b g_{ad} - \widehat{\nabla}_d g_{ab} \right)} \tag{B.5}$$

This choice of $\mathfrak{C}^c{}_{ab}$ is manifestly unique; note that in the special case when $\widehat{\nabla}_a$ is the ordinary partial derivative ∂_a, then $\mathfrak{C}^c{}_{ab}$ is simply the Christoffel symbol $\Gamma^c{}_{ab}$.

Having now a well defined relation between connections, we may compare their curvature. Recall the Ricci identity of the Riemann tensor: for any one-form ω_d, [2]

$$2\nabla_{[a}\nabla_{b]}\omega_c = R_{abc}{}^d \omega_d. \tag{B.6}$$

We then apply (B.1) to this expression; consider the first term on the LHS of (B.6):

$$\begin{aligned}
\nabla_a \nabla_b \omega_c &= \nabla_a (\nabla_b \omega_c) \\
&= \nabla_a \left(\widehat{\nabla}_b \omega_c - \mathfrak{C}^d{}_{bc} \omega_d \right) \\
&= \nabla_a \left(\widehat{\nabla}_b \omega_c \right) - \nabla_a \left(\mathfrak{C}^d{}_{bc} \omega_d \right) \\
&= \widehat{\nabla}_a \widehat{\nabla}_b \omega_c - \mathfrak{C}^d{}_{ab} \widehat{\nabla}_d \omega_c - \mathfrak{C}^d{}_{ac} \widehat{\nabla}_b \omega_d \\
&\quad - \widehat{\nabla}_a \left(\mathfrak{C}^d{}_{bc} \omega_d \right) + \mathfrak{C}^d{}_{ec}\, \mathfrak{C}^e{}_{ab}\, \omega_d + \mathfrak{C}^d{}_{eb}\, \mathfrak{C}^e{}_{ac}\, \omega_d \\
&= \widehat{\nabla}_a \widehat{\nabla}_b \omega_c - \mathfrak{C}^d{}_{ab} \widehat{\nabla}_d \omega_c - \mathfrak{C}^d{}_{ac} \widehat{\nabla}_b \omega_d \\
&\quad - \mathfrak{C}^d{}_{bc}\, \widehat{\nabla}_a \omega_d - \omega_d\, \widehat{\nabla}_a \mathfrak{C}^d{}_{bc} + \mathfrak{C}^d{}_{ec}\, \mathfrak{C}^e{}_{ab}\, \omega_d + \mathfrak{C}^d{}_{eb}\, \mathfrak{C}^e{}_{ac}\, \omega_d.
\end{aligned}$$

Then permuting $a \leftrightarrow b$ and subtracting,

$$\begin{aligned}
2\nabla_{[a}\nabla_{b]}\omega_c &= \widehat{\nabla}_a \widehat{\nabla}_b \omega_c - \mathfrak{C}^d{}_{ab} \widehat{\nabla}_d \omega_c - \mathfrak{C}^d{}_{ac} \widehat{\nabla}_b \omega_d \\
&\quad - \mathfrak{C}^d{}_{bc}\, \widehat{\nabla}_a \omega_d - \omega_d\, \widehat{\nabla}_a \mathfrak{C}^d{}_{bc} + \mathfrak{C}^d{}_{ec}\, \mathfrak{C}^e{}_{ab}\, \omega_d + \mathfrak{C}^d{}_{eb}\, \mathfrak{C}^e{}_{ac}\, \omega_d \\
&\quad - \widehat{\nabla}_b \widehat{\nabla}_a \omega_c + \mathfrak{C}^d{}_{ab} \widehat{\nabla}_d \omega_c + \mathfrak{C}^d{}_{bc} \widehat{\nabla}_a \omega_d \\
&\quad + \mathfrak{C}^d{}_{ac}\, \widehat{\nabla}_b \omega_d + \omega_d\, \widehat{\nabla}_b \mathfrak{C}^d{}_{ac} - \mathfrak{C}^d{}_{ec}\, \mathfrak{C}^e{}_{ab}\, \omega_d - \mathfrak{C}^d{}_{ea}\, \mathfrak{C}^e{}_{bc}\, \omega_d. \\
&= \underbrace{2\, \widehat{\nabla}_{[a} \widehat{\nabla}_{b]} \omega_c}_{= \widehat{R}_{abc}{}^d \omega_d} - 2\, \widehat{\nabla}_{[a} \mathfrak{C}^d{}_{b]c} \omega_d + 2\, \mathfrak{C}^e{}_{c[a}\, \mathfrak{C}^d{}_{b]e} \omega_d \\
&= \widehat{R}_{abc}{}^d \omega_d - 2\, \widehat{\nabla}_{[a} \mathfrak{C}^d{}_{b]c} \omega_d + 2\, \mathfrak{C}^e{}_{c[a}\, \mathfrak{C}^d{}_{b]e} \omega_d.
\end{aligned}$$

This relation holds for any one-form ω_d; thus we have found a transformation law for the Riemann tensor from a connection ∇ to a connection $\widehat{\nabla}$:

$$R_{abc}{}^d = \widehat{R}_{abc}{}^d - 2\, \widehat{\nabla}_{[a} \mathfrak{C}^d{}_{b]c} + 2\, \mathfrak{C}^e{}_{c[a}\, \mathfrak{C}^d{}_{b]e}. \tag{B.7}$$

Similarly, contracting $b = d$, we get a relation for the Ricci tensor:

$$R_{ac} = \widehat{R}_{ac} - 2\, \widehat{\nabla}_{[a} \mathfrak{C}^b{}_{b]c} + 2\, \mathfrak{C}^e{}_{c[a}\, \mathfrak{C}^b{}_{b]e}. \tag{B.8}$$

[2] You may check that this expression for the Ricci identity is entirely equivalent to (1.22). Here $R_{abc}{}^d$ is obtained from the usual coordinate expression of the Riemann tensor $R^d{}_{abc}$ by performing some straightforward index gymnastics and using the known symmetries of the Riemann tensor ($R_{abc}{}^d = g^{de} R_{abce} = g^{de} R_{ceab} = -g^{de} R_{ecab} = -R^d{}_{cab} = R^d{}_{cba}$).

Then, if the conformal scaling of the metric is such that

$$\begin{aligned}\widehat{g}_{ab} &= \chi g_{ab}\\ \widehat{g}^{ab} &= \chi^{-1} g^{ab},\end{aligned}$$

(as it shall be in our case), then we can get a transformation law for the Ricci scalar as well by raising an index on (B.8) and contracting:

$$\begin{aligned}g^{ac}R_{ac} &= g^{ac}\left(\widehat{R}_{ac} - 2\,\widehat{\nabla}_{[a}\mathfrak{C}^{b}{}_{b]c} + 2\,\mathfrak{C}^{e}{}_{c[a}\,\mathfrak{C}^{b}{}_{b]e}\right)\\ R &= \chi\widehat{g}^{ac}\left(\widehat{R}_{ac} - 2\,\widehat{\nabla}_{[a}\mathfrak{C}^{b}{}_{b]c} + 2\,\mathfrak{C}^{e}{}_{c[a}\,\mathfrak{C}^{b}{}_{b]e}\right)\\ &= \chi\left(\widehat{R} - 2\,\widehat{g}^{ac}\widehat{\nabla}_{[a}\mathfrak{C}^{b}{}_{b]c} + 2\,\widehat{g}^{ac}\mathfrak{C}^{e}{}_{c[a}\,\mathfrak{C}^{b}{}_{b]e}\right).\end{aligned}$$

We summarize these three key curvature transformations here,

$$\boxed{\begin{aligned}R_{abc}{}^{d} &= \widehat{R}_{abc}{}^{d} - 2\,\widehat{\nabla}_{[a}\mathfrak{C}^{d}{}_{b]c} + 2\,\mathfrak{C}^{e}{}_{c[a}\,\mathfrak{C}^{d}{}_{b]e}\\ R_{ab} &= \widehat{R}_{ab} - 2\,\widehat{\nabla}_{[a}\mathfrak{C}^{c}{}_{c]b} + 2\,\mathfrak{C}^{e}{}_{b[a}\,\mathfrak{C}^{c}{}_{c]e}\\ R &= \chi\left(\widehat{R} - 2\,\widehat{g}^{ab}\widehat{\nabla}_{[a}\mathfrak{C}^{c}{}_{c]b} + 2\,\widehat{g}^{ab}\mathfrak{C}^{e}{}_{b[a}\,\mathfrak{C}^{c}{}_{c]e}\right)\end{aligned}}\qquad \begin{aligned}&\text{(B.9a)}\\&\text{(B.9b)}\\&\text{(B.9c)}\end{aligned}$$

These are very important transformation laws that we will use quite often in the main text…In fact, let us use them now to write the conformal decomposition of both the 3D (spatial) Ricci tensor R_{ij} and Ricci scalar R that we are using in our treatment: We start by calculating the $\mathfrak{C}^{c}{}_{ab}$ relation between our two connections D and $\bar{D}$, using (B.5):

$$\begin{aligned}\mathfrak{C}^{k}{}_{ij} &= \frac{1}{2}\gamma^{k\ell}\left(\bar{D}_i\gamma_{j\ell} + \bar{D}_j\gamma_{i\ell} - \bar{D}_k\gamma_{ij}\right)\\ &= \frac{1}{2}\chi\bar{\gamma}^{k\ell}\left(\bar{D}_i(\chi^{-1}\bar{\gamma}_{j\ell}) + \bar{D}_j(\chi^{-1}\bar{\gamma}_{i\ell}) - \bar{D}_\ell(\chi^{-1}\bar{\gamma}_{ij})\right)\\ &= \frac{1}{2}\chi\bar{\gamma}^{k\ell}(\chi^{-1}\underbrace{\bar{D}_i\bar{\gamma}_{j\ell}}_{=0} + \bar{\gamma}_{j\ell}\,\bar{D}_i\chi^{-1} + \chi^{-1}\underbrace{\bar{D}_j\bar{\gamma}_{i\ell}}_{=0} + \bar{\gamma}_{i\ell}\,\bar{D}_j\chi^{-1} - \chi^{-1}\underbrace{\bar{D}_\ell\bar{\gamma}_{ij}}_{=0} - \bar{\gamma}_{ij}\,\bar{D}_\ell\chi^{-1})\\ &= \frac{1}{2}\chi\bar{\gamma}^{k\ell}\left(-\chi^{-2}\bar{\gamma}_{j\ell}\,\bar{D}_i\chi - \chi^{-2}\bar{\gamma}_{i\ell}\,\bar{D}_j\chi + \chi^{-2}\bar{\gamma}_{ij}\,\bar{D}_\ell\chi\right)\\ &= \frac{1}{2}\chi^{-1}\left(\bar{\gamma}_{ij}\,\bar{D}^k\chi - 2\,\delta_{(i}{}^{k}\,\bar{D}_{j)}\chi\right)\\ &= \frac{1}{2}\bar{\gamma}_{ij}\,\bar{D}^k(\log\chi) - \delta_{(i}{}^{k}\,\bar{D}_{j)}(\log\chi).\end{aligned}\qquad\text{(B.10)}$$

Also, in terms of ψ (we will use this when dealing with the initial data problem (see Chapter 3)),

$$\begin{aligned}\mathfrak{C}^{k}{}_{ij} &= \frac{1}{2}\gamma^{k\ell}\left(\bar{D}_i\gamma_{j\ell} + \bar{D}_j\gamma_{i\ell} - \bar{D}_k\gamma_{ij}\right)\\ &= \frac{1}{2}\psi^{-4}\bar{\gamma}^{k\ell}\left(\bar{D}_i(\psi^4\bar{\gamma}_{j\ell}) + \bar{D}_j(\psi^4\bar{\gamma}_{i\ell}) - \bar{D}_\ell(\psi^4\bar{\gamma}_{ij})\right)\\ &= \frac{1}{2}\psi^{-4}\bar{\gamma}^{k\ell}\left(4\psi^3\bar{\gamma}_{j\ell}\,\bar{D}_i\psi + 4\psi^3\bar{\gamma}_{i\ell}\,\bar{D}_j\psi - 4\psi^3\bar{\gamma}_{ij}\,\bar{D}_\ell\psi\right)\\ &= 2\psi^{-1}\bar{\gamma}^{k\ell}\left(\bar{\gamma}_{j\ell}\,\bar{D}_i\psi + \bar{\gamma}_{i\ell}\,\bar{D}_j\psi - \bar{\gamma}_{ij}\,\bar{D}_\ell\psi\right)\\ &= 2\bar{\gamma}^{k\ell}\left(\bar{\gamma}_{j\ell}\,\bar{D}_i(\log\psi) + \bar{\gamma}_{i\ell}\,\bar{D}_j(\log\psi) - \bar{\gamma}_{ij}\,\bar{D}_\ell(\log\psi)\right)\\ &= 4\delta_{(i}{}^{k}\,\bar{D}_{j)}(\log\psi) - 2\bar{\gamma}_{ij}\,\bar{D}^k(\log\psi).\end{aligned}\qquad\text{(B.11)}$$

We now apply (B.10) to (B.9b) and expand:

$$
\begin{aligned}
R_{ij} &= \bar{R}_{ij} - 2\,\bar{D}_{[i}\mathfrak{C}^{k}{}_{k]j} + 2\,\mathfrak{C}^{\ell}{}_{j[i}\,\mathfrak{C}^{k}{}_{k]\ell} \\
&= \bar{R}_{ij} - \left(\bar{D}_i\mathfrak{C}^{k}{}_{jk} - \bar{D}_k\mathfrak{C}^{k}{}_{ij}\right) + \left(\mathfrak{C}^{\ell}{}_{ij}\,\mathfrak{C}^{k}{}_{\ell k} - \mathfrak{C}^{\ell}{}_{jk}\,\mathfrak{C}^{k}{}_{i\ell}\right) \\
&= \bar{R}_{ij} - \bar{D}_i\left[\frac{1}{2}\bar{\gamma}_{jk}\,\bar{D}^k(\log\chi) - \delta_{(j}{}^{k}\,\bar{D}_{k)}(\log\chi)\right] \\
&\quad + \bar{D}_k\left[\frac{1}{2}\bar{\gamma}_{ij}\,\bar{D}^k(\log\chi) - \delta_{(i}{}^{k}\,\bar{D}_{j)}(\log\chi)\right] \\
&\quad + \left[\frac{1}{2}\bar{\gamma}_{ij}\,\bar{D}^\ell(\log\chi) - \delta_{(i}{}^{\ell}\,\bar{D}_{j)}(\log\chi)\right]\left[\frac{1}{2}\bar{\gamma}_{\ell k}\,\bar{D}^k(\log\chi) - \delta_{(\ell}{}^{k}\,\bar{D}_{k)}(\log\chi)\right] \\
&\quad - \left[\frac{1}{2}\bar{\gamma}_{jk}\,\bar{D}^\ell(\log\chi) - \delta_{(j}{}^{\ell}\,\bar{D}_{k)}(\log\chi)\right]\left[\frac{1}{2}\bar{\gamma}_{i\ell}\,\bar{D}^k(\log\chi) - \delta_{(i}{}^{k}\,\bar{D}_{\ell)}(\log\chi)\right] \\
&= \bar{R}_{ij} - \frac{1}{2}\bar{D}_i\bar{D}_j(\log\chi) + \frac{1}{2}\bar{D}_i\bar{D}_j(\log\chi) + \frac{3}{2}\bar{D}_i\bar{D}_j(\log\chi) \\
&\quad + \frac{1}{2}\bar{\gamma}_{ij}\,\bar{D}_k\bar{D}^k(\log\chi) - \frac{1}{2}\bar{D}_i\bar{D}_j(\log\chi) - \frac{1}{2}\underbrace{\bar{D}_j\bar{D}_i(\log\chi)}_{=\,\bar{D}_i\bar{D}_j(\log\chi)\text{ since }\log\chi\text{ is a scalar}} \\
&\quad + \frac{1}{4}\bar{\gamma}_{ij}\,\bar{D}_k(\log\chi)\bar{D}^k(\log\chi) - \frac{1}{4}\bar{\gamma}_{ij}\,\bar{D}_k(\log\chi)\bar{D}^k(\log\chi) - \frac{3}{4}\bar{\gamma}_{ij}\,\bar{D}_k(\log\chi)\bar{D}^k(\log\chi) \\
&\qquad - \frac{1}{4}\bar{D}_i(\log\chi)\bar{D}_j(\log\chi) - \frac{1}{4}\bar{D}_i(\log\chi)\bar{D}_j(\log\chi) + \frac{1}{4}\bar{D}_i(\log\chi)\bar{D}_j(\log\chi) \\
&\qquad + \frac{3}{4}\bar{D}_i(\log\chi)\bar{D}_j(\log\chi) + \frac{3}{4}\bar{D}_i(\log\chi)\bar{D}_j(\log\chi) + \frac{1}{4}\bar{D}_i(\log\chi)\bar{D}_j(\log\chi) \\
&\quad - \frac{1}{4}\bar{D}_i(\log\chi)\bar{D}_j(\log\chi) + \frac{1}{4}\bar{\gamma}_{ij}\,\bar{D}_k(\log\chi)\bar{D}^k(\log\chi) + \frac{1}{4}\bar{D}_i(\log\chi)\bar{D}_j(\log\chi) \\
&\qquad + \frac{1}{4}\bar{\gamma}_{ij}\,\bar{D}_k(\log\chi)\bar{D}^k(\log\chi) - \frac{1}{4}\bar{D}_i(\log\chi)\bar{D}_j(\log\chi) - \frac{1}{4}\bar{D}_i(\log\chi)\bar{D}_j(\log\chi) \\
&\qquad + \frac{1}{4}\bar{D}_i(\log\chi)\bar{D}_j(\log\chi) - \frac{1}{4}\bar{D}_i(\log\chi)\bar{D}_j(\log\chi) - \frac{3}{4}\bar{D}_i(\log\chi)\bar{D}_j(\log\chi) \\
&= \bar{R}_{ij} + \frac{1}{2}\left(\bar{D}_i\bar{D}_j(\log\chi) + \bar{\gamma}_{ij}\,\bar{D}_k\bar{D}^k(\log\chi)\right) + \frac{1}{4}\left(\bar{D}_i(\log\chi)\bar{D}_j(\log\chi) - \bar{\gamma}_{ij}\,\bar{D}_k(\log\chi)\bar{D}^k(\log\chi)\right).
\end{aligned}
$$

Thus we have found that the 3D Ricci tensor can be split as

$$
\boxed{
\begin{aligned}
R_{ij} &= \bar{R}_{ij} + R^{\chi}_{ij} && \text{(B.12a)} \\
\bar{R}_{ij} &= \partial_k\bar{\Gamma}^k_{ij} - \partial_j\bar{\Gamma}^k_{ik} + \bar{\Gamma}^k_{\ell k}\,\bar{\Gamma}^\ell_{ij} - \bar{\Gamma}^k_{\ell j}\,\bar{\Gamma}^\ell_{ik} && \text{(B.12b)} \\
R^{\chi}_{ij} &= \frac{1}{2}\left(\bar{D}_i\bar{D}_j(\log\chi) + \bar{\gamma}_{ij}\,\bar{D}_k\bar{D}^k(\log\chi)\right) && \text{(B.12c)} \\
&\quad + \frac{1}{4}\left(\bar{D}_i(\log\chi)\bar{D}_j(\log\chi) - \bar{\gamma}_{ij}\,\bar{D}_k(\log\chi)\bar{D}^k(\log\chi)\right)
\end{aligned}
}
$$

Then, raising an index and contracting, we get

$$
\begin{aligned}
\gamma^{ij}R_{ij} &= \gamma^{ij}\left(\bar{R}_{ij} + R^{\chi}_{ij}\right) = \chi\bar{\gamma}^{ij}\left(\bar{R}_{ij} + R^{\chi}_{ij}\right) \\
R &= \chi\bar{R} + \chi[\frac{1}{2}\left(\bar{D}_k\bar{D}^k(\log\chi) + 3\,\bar{D}_k\bar{D}^k(\log\chi)\right) \\
&\quad + \frac{1}{4}\left(\bar{D}_k(\log\chi)\bar{D}^k(\log\chi) - 3\,\bar{D}_k(\log\chi)\bar{D}^k(\log\chi)\right)] \\
&\quad = \chi\bar{R} + 2\,\chi\bar{D}_k\bar{D}^k(\log\chi) - \frac{1}{2}\,\chi\bar{D}_k(\log\chi)\bar{D}^k(\log\chi).
\end{aligned}
$$

Hence we have derived a conformal decomposition for the Ricci scalar as well,

$$
\boxed{R = \chi\bar{R} + 2\,\chi\bar{D}^2(\log\chi) - \frac{1}{2}\,\chi\bar{D}_k(\log\chi)\bar{D}^k(\log\chi)} \tag{B.13}
$$

where $\bar{D}^2 = \bar{D}_k\bar{D}^k$ the conformal Laplace operator. We may further expand this expression as follows:

$$\begin{aligned}
R &= \chi\bar{R} + 2\,\chi\bar{\gamma}^{ij}\bar{D}_i(\bar{D}_j(\log\chi)) - \frac{1}{2}\,\chi\bar{\gamma}^{ij}\bar{D}_i(\log\chi)\bar{D}_j(\log\chi) \\
&= \chi\bar{R} + 2\,\chi\bar{\gamma}^{ij}\bar{D}_i(\chi^{-1}\bar{D}_j\chi) - \frac{1}{2}\,\chi\cdot\chi^{-2}\bar{\gamma}^{ij}\bar{D}_i\chi\bar{D}_j\chi \\
&= \chi\bar{R} + 2\,\chi\bar{\gamma}^{ij}\left(\chi^{-1}\bar{D}_i\bar{D}_j\chi - \chi^{-2}\bar{D}_i\chi\bar{D}_j\chi\right) - \frac{1}{2}\,\chi^{-1}\bar{D}_k\chi\bar{D}^k\chi \\
&= \chi\bar{R} + 2\,\bar{D}^2\chi - \frac{5}{2}\,\chi^{-1}\bar{D}_k\chi\bar{D}^k\chi.
\end{aligned} \tag{B.14}$$

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