Part III Gravitational Waves and Numerical Relativity

Lecture Notes

Abstract

This document contains the long version of the lecture notes for the Part III course *Gravitational Waves and Numerical Relativity.* These notes are extensive and written such that they can be consumed either together with the lecture or on their own.

These notes assume that readers are already familiar with general relativity as lectured, for example, in DAMTP's Part II and Part III General Relativity lectures. Some knowledge of Part III Black Holes will be helpful, in particular a basic knowledge of the properties of the Kerr spacetime describing rotating black holes. We will also introduce some background material on the structure and properties of partial differential equations, but this should be consumable with a background in standard mathematical methods as lectured in Part IB without requiring exposure to specialized lectures dedicated to partial differential equations. There exists by now a healthy amount of text books and lecture style notes where the reader will find more in-depth discussion of some of our topics; knowledge of this literature is, however, not anticipated in our lecture.

- M. Alcubierre, *Introduction to 3+1 Numerical Relativity.* Oxford University Press (2008)
- T. W. Baumgarte, and S. L. Shapiro, *Numerical Relativity.* Cambridge University Press (2010)
- T. W. Baumgarte, and S. L. Shapiro, *Numerical Relativity – Starting from Scratch.* Cambridge University Press (2021)
- R. LeVeque, *Numerical methods for conservation laws.* Birkhäuser Verlag (1992)
- R, Courant, D. Hilbert, *Methods of Mathematical Physics II.* Wiley-Interscience, New York (1962).
- E. Gourgoulhon, *3+1 Formalism and Bases of Numerical Relativity*, Springer, New York (2012); see also `https://arxiv.org/abs/gr-qc/0703035`.
- M. Maggiore, *Gravitational Waves, Vol. 1: Theory and Experiments*, Oxford University Press (2007); *Gravitational Waves Vol. 2: Astrophysics and Cosmology*", Oxford University Press (2018).
- R. d'Inverno, "Introducing Einstein's Relativity", Clarendon Press, Oxford (1992).

Example sheets will be made available on

`http://www.damtp.cam.ac.uk/user/examples`

Lectures Webpage:

`http://www.damtp.cam.ac.uk/user/us248/Lectures/lectures.html`

This course does not involve practical coding in numerical relativity, but readers interested in an open-source numerical relativity code in spherical symmetry are recommended to explore Katy Clough's `Engrenage` [1].

Acknowledgments: To be added...

Cambridge, 25 Apr 2022

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Contents

A Introduction and conventions

A.1 Introduction and motivation

These lecture notes are concerned with the Einstein field equations of general relativity. From a physical point of view, our main goal is to understand the phenomenon of gravitational waves and to discuss the computational methods that enable us to determine the gravitational-wave patterns emitted by the most common types of astrophysical sources. The only method presently available for solving the Einstein equations in the fully non-linear regime for generic physical systems consists in numerical simulations. This, in turn, requires us to write the Einstein equations in a form suitable for computer modeling. This turns out quite a subtle issue and again requires us to look in detail at the structure of the Einstein equations.

We will have to take some care in organizing our journey through these topics to make sure we always maintain a clear view of the overall picture. We will begin with a brief overview of the Einstein equations and our specific choice of conventions. This will be followed by the canonical analysis of gravitational waves using the linearized field equations. While this analysis had already been noticed by Einstein in 1918 [2], its interpretation has been the subject of controversy for about 40 years thereafter. Even Einstein himself called into question the existence of gravitational waves. How could such confusion arise inside a concrete theory formulated in a clear and rigorous mathematical language? As we have already seen in the Part II and Part III lectures on General Relativity and Black Holes, the interpretation of solutions to the Einstein equations faces multiple complications not present in Newtonian physics, such as the coordinate or gauge freedom and a lack of concrete definitions for local mass and energy. Here, we are facing the additional problem of non-linearity; it is far from clear whether solutions of the linearized equations represent good approximations of weak-field solutions to the fully non-linear theory. A fully non-linear treatment of wave like solutions in general relativity is much harder and was only achieved around 1960 with the seminal work by Bondi, Sachs and collaborators [3, 4] using the characteristic formulation of the Einstein equations. This guides us to the next stage of these notes, a brief discussion of the classification of partial differential equations and their characteristic structure, followed by a first analysis of the Einstein equations and the Bondi-Sachs formalism itself.

In spite of the elegance of the characteristic formalism, the vast majority of computational modeling of astrophysical sources inside the framework of general relativity proceeds inside a so-called space-time or 3+1 split. The comprehensive development of such a 3+1 formalism of Einstein's equations is another result that has only been obtained decades after the theory itself, mainly in the form of the canonical formulation by Arnowitt, Deser and Misner [5] and York's reformulation [6]. And yet, even these developments were not enough to facilitate fully functional numerical simulations. For one thing, the resulting equations turn out to be ill-posed in a sense we will make more concrete later on and, second, it is critical to employ the coordinate freedom of general relativity in a way that prevents simulations from running into the singularities inherent to Einstein's theory. Indeed, the two-body problem of general relativity, the inspiral and merger of two black holes, remained unsolved until Pretorius' 2005 breakthrough [7], followed and confirmed about half a year later by the so-called *moving punc-*

ture simulations of the Brownsville and NASA Goddard groups [8, 9]; see also [10] for a review. Rapid improvements in the codes' efficiency and accuracy led to more precise gravitational-wave calculations in the following years; and not too soon, as these turned out critical in the Nobel-Prize winning direct detection of a gravitational-wave signal by LIGO in 2015 [11]. The second half of these lectures will guide us through the theoretical foundations of these calculations: the 3+1 formalism of general relativity, the remedies applied to it for obtaining a well-posed formulation and the eventual extraction of theoretical predictions for gravitational waveforms as used in the ongoing gravitational-wave observation programs using the LIGO, Virgo and KAGRA detectors as well as future observatories.

We will try to not overwhelm readers with too many acronyms, but some are so common and convenient that we give in to the temptation of using them in the remainder of these notes. Here is a brief glossary for orientation[1].

Glossary

ADM	Arnowitt-Deser-Misner
BH	black hole
GR	general relativity
GW	gravitational wave
KAGRA	Kamioka Gravitational Wave Detector
LIGO	Laser Interferometer Gravitational-Wave Observatory
PDE	Partial differential equation

A.2 Definitions and conventions

Einstein's theory of general relativity models spacetimes as four-dimensional Lorentzian manifolds, i.e. four-dimensional manifolds $\mathcal{M}$ equipped with a metric $g_{\alpha\beta}$ of signature +2, where we employ a "mostly positive" signature $-+++$, i.e. timelike (spacelike) vectors have negative (positive) norm. In these notes, we follow the conventions of Misner, Thorne and Wheeler [12]) given by the following definitions for the quantities derived from the spacetime metric. We use Greek letters α, β, ... for spacetime indices running from 0 to 3 and, further below, we shall be using middle to late Latin letters i, j, ... for spatial indices running from 1 to 3.

[1]"Virgo" is not an acronym but simply the name of the gravitational-wave detector near Pisa in Italy.

Def. : On a Lorentzian manifold $\mathcal{M}$ with metric $g_{\alpha\beta}$ of signature $+2$, we define the

$$\begin{aligned}
&\textit{Levi-Civita connection:} && \Gamma^{\mu}_{\beta\gamma} := \frac{1}{2} g^{\mu\rho} \left(\partial_\beta g_{\gamma\rho} + \partial_\gamma g_{\rho\beta} - \partial_\rho \gamma_{\beta\gamma} \right) \,, \\
&\textit{Riemann tensor:} && R^{\gamma}{}_{\rho\alpha\beta} := \partial_\alpha \Gamma^{\gamma}_{\rho\beta} - \partial_\beta \Gamma^{\gamma}_{\rho\alpha} + \Gamma^{\mu}_{\rho\beta}\Gamma^{\gamma}_{\mu\alpha} - \Gamma^{\mu}_{\rho\alpha}\Gamma^{\gamma}_{\mu\beta} \,, \\
&\textit{Ricci tensor and scalar:} && R_{\alpha\beta} := R^{\mu}{}_{\alpha\mu\beta} \,, \qquad R := R^{\mu}{}_{\mu} \,, \\
&\textit{Einstein tensor:} && G_{\alpha\beta} := R_{\alpha\beta} - \frac{1}{2} g_{\alpha\beta} R \,.
\end{aligned} \tag{A.1}$$

Proposition: The Riemann and Einstein tensors satisfy the

$$\textit{Bianchi identities:} \qquad R^{\mu}{}_{\nu[\rho\sigma;\lambda]} = \nabla_{[\lambda|} R^{\mu}{}_{\nu|\rho\sigma]} = 0 \,, \tag{A.2}$$

$$\textit{Contracted Bianchi identities:} \qquad \nabla^{\mu} G_{\mu\alpha} = 0 \,. \tag{A.3}$$

These identities follow from the symmetry of the Riemann tensor and their derivation can be found, for example, in Reall's Part III lecture notes [13]. The Einstein equations are then given by

$$G_{\alpha\beta} = \frac{8\pi G}{c^4} T_{\alpha\beta} = 8\pi T_{\alpha\beta} \,, \tag{A.4}$$

where we have temporarily restored (and then quickly dropped) Newton's gravitational constant G and the speed of light c. Henceforth we will set $G = 1 = c$ in our equations unless otherwise stated. The energy-momentum tensor $T_{\alpha\beta}$ needs to be specified separately, depending on the type of matter under consideration. In vacuum, we have $T_{\alpha\beta} = 0$ and, hence, $G^{\mu}{}_{\mu} = -R = 0$, so that the Einstein equations in vacuum become

$$R_{\alpha\beta} = 0 \,. \tag{A.5}$$

B Linearized theory and gravitational waves

B.1 The linearized Einstein equations

Perturbation theory plays an important role in many areas of physics and general relativity is no exception. Furthermore, gauge invariant perturbation theory in general relativity leads to a remarkably elegant formalism developed by Gerlach and Sengupta [14, 15]. Readers may also find Chandrasekar's book [16] a good starting reference for a more in-depth exploration of black-hole perturbation theory. Here, we restrict ourselves to the specific case of small perturbations around Minkowski spacetime in Cartesian coordinates, i.e. the manifold $\mathcal{M} = \mathbb{R}^4$ with metric

$$g_{\alpha\beta} = \eta_{\alpha\beta} = \mathrm{diag}(-1,\ 1,\ 1,\ 1)\,. \tag{B.1}$$

The perturbations are then given by a tensor field $h_{\alpha\beta} = \mathcal{O}(\epsilon) \ll 1$ on the Minkowski background. The parameter ϵ represents some small dimensionless number that will serve us in our book keeping throughout this section. In practice, this number represents some physical quantity or, more commonly, the ratio of some physical quantities. For example, in weak-field calculations in the solar system, this parameter may denote the ratio of the solar mass to the distance from the sun, say the (average) radius of Mercury's orbit. In a sense that we will make more concrete as we proceed with our calculations, we may indeed regard $h_{\alpha\beta}$ as a genuine tensor field in the Minkowski spacetime. Note that we thus have two metrics, the background metric $\eta_{\alpha\beta}$ and the physical metric

$$g_{\alpha\beta} = \eta_{\alpha\beta} + h_{\alpha\beta}\,. \tag{B.2}$$

The inverse physical metric $g^{\alpha\beta}$ is given by an as yet unknown perturbation of the inverse background metric $\eta^{\alpha\beta}$,

$$g^{\alpha\beta} = \eta^{\alpha\beta} + k^{\alpha\beta}\,, \qquad \text{where} \qquad k^{\alpha\beta} = \mathcal{O}(\epsilon)\,, \tag{B.3}$$

and is defined by the condition $g^{\alpha\mu}g_{\mu\beta} = \delta^{\alpha}{}_{\beta}$. At linear order this gives us

$$\begin{aligned}
g^{\alpha\mu}g_{\mu\beta} &= (\eta^{\alpha\mu} + k^{\alpha\mu})(\eta_{\mu\beta} + h_{\mu\beta}) = \eta^{\alpha\mu}\eta_{\mu\beta} + \eta^{\alpha\mu}h_{\mu\beta} + k^{\alpha\mu}\eta_{\mu\beta} + \underbrace{k^{\alpha\mu}h_{\mu\beta}}_{=\mathcal{O}(\epsilon^2)\to 0} \\
&= \delta^{\alpha}{}_{\beta} + \eta^{\alpha\mu}h_{\mu\beta} + k^{\alpha\mu}\eta_{\mu\beta} \overset{!}{=} \delta^{\alpha}{}_{\beta} \qquad \Big|\ \cdot\,\eta^{\gamma\beta} \\
\Rightarrow\quad k^{\alpha\gamma} &= -\eta^{\gamma\beta}\eta^{\alpha\mu}h_{\mu\beta} =: -h^{\alpha\gamma}\,.
\end{aligned} \tag{B.4}$$

In the last step, we have introduced the convention that we raise and lower indices with the background metric. It is in this sense, that we regard the tensor field $h_{\mu\nu}$ as a tensor field on the Minkowski background.

In a similar way, we can compute all derived quantities of the physical metric in terms of the background metric and the perturbations. The key simplification of linearized theory is that we can discard as negligible at any stage terms of order $\mathcal{O}(\epsilon^2)$ or higher. We thus find

$$\Gamma^{\mu}_{\nu\rho} = \frac{1}{2}\eta^{\mu\sigma}(\partial_\rho h_{\sigma\nu} + \partial_\nu h_{\rho\sigma} - \partial_\sigma h_{\nu\rho})\,, \tag{B.5}$$

$$R_{\mu\nu\rho\sigma} = \frac{1}{2}(\partial_\rho\partial_\nu h_{\mu\sigma} + \partial_\sigma\partial_\mu h_{\nu\rho} - \partial_\rho\partial_\mu h_{\nu\sigma} - \partial_\sigma\partial_\nu h_{\mu\rho})\,, \tag{B.6}$$

$$R_{\mu\nu} = \partial^\rho\partial_{(\mu}h_{\nu)\rho} - \frac{1}{2}\partial^\rho\partial_\rho h_{\mu\nu} - \partial_\mu\partial_\nu h\,, \qquad \text{where} \qquad h := h^\mu{}_\mu\,, \quad \partial^\mu := \eta^{\mu\rho}\partial_\rho\,, \tag{B.7}$$

$$G_{\mu\nu} = \partial^\rho\partial_{(\mu}h_{\nu)\rho} - \frac{1}{2}\partial^\rho\partial_\rho h_{\mu\nu} - \partial_\mu\partial_\nu h - \frac{1}{2}\eta_{\mu\nu}(\partial^\rho\partial^\sigma h_{\rho\sigma} - \partial^\rho\partial_\rho h)\,. \tag{B.8}$$

These equations may not look too informative, but we can already derive two important properties that will be important later on. First, note that the second term on the right-hand side of Eq. (B.7) for the Ricci tensor represents the wave operator acting on $h_{\mu\nu}$. Likewise, Eq. (B.8) contains two wave operators. Wave operators are nice in the sense that they lead to manifestly hyperbolic partial differential equations as we will see in Sec. C below. Much of our following calculations serve the purpose of getting rid of all the other second derivatives in the expressions for $R_{\mu\nu}$ and $G_{\mu\nu}$ such that we end up with a wave equation for $h_{\mu\nu}$. The second observation arises from plugging Eq. (B.8) into the Einstein equations $G_{\mu\nu} = 8\pi T_{\mu\nu}$. Since $G_{\mu\nu} = \mathcal{O}(\epsilon)$, we immediately conclude that the local matter distribution is weak, $T_{\mu\nu} = \mathcal{O}(\epsilon)$.

Def. : The *trace-reversed metric perturbation* is defined as

$$\bar{h}_{\mu\nu} := h_{\mu\nu} - \frac{1}{2}h\eta_{\mu\nu} \quad \Rightarrow \quad \bar{h} = \bar{h}^\mu{}_\mu = -h \quad \Rightarrow \quad h_{\mu\nu} = \bar{h}_{\mu\nu} - \frac{1}{2}\bar{h}\eta_{\mu\nu}\,. \tag{B.9}$$

A straightforward calculation shows that this shortens Eq. (B.8) to

$$G_{\mu\nu} = -\frac{1}{2}\partial^\rho\partial_\rho\bar{h}_{\mu\nu} + \partial^\rho\partial_{(\mu}\bar{h}_{\nu)\rho} - \frac{1}{2}\eta_{\mu\nu}\partial^\rho\partial^\sigma\bar{h}_{\rho\sigma} = 8\pi T_{\mu\nu}\,. \tag{B.10}$$

We can achieve further simplification by changing to a more suitable set of coordinates. In this process, however, we would like to preserve the background metric and therefore consider coordinate transformations at perturbative level. These are given by a "flow vector field" $\xi^\mu = \mathcal{O}(\epsilon)$ and define new coordinates according to

$$\tilde{x}^\alpha = x^\alpha - \xi^\alpha \qquad \Leftrightarrow \qquad x^\alpha = \tilde{x}^\alpha + \xi^\alpha\,. \tag{B.11}$$

The metric in the new coordinate system becomes

$$\begin{aligned} \tilde{g}_{\alpha\beta} &= \frac{\partial x^\mu}{\partial\tilde{x}^\alpha}\frac{\partial x^\nu}{\partial\tilde{x}^\beta}g_{\mu\nu} = g_{\alpha\beta} + \partial_\alpha\xi^\mu\delta^\nu{}_\beta g_{\mu\nu} + \partial_\beta\xi^\nu\delta^\mu{}_\alpha g_{\mu\nu} + \mathcal{O}(\epsilon^2) \\ &= \eta_{\alpha\beta} + h_{\alpha\beta} + \partial_\alpha\xi_\beta + \partial_\beta\xi_\alpha + \mathcal{O}(\epsilon^2)\,, \end{aligned} \tag{B.12}$$

so that the perturbation transforms according to

$$\begin{aligned} & h_{\alpha\beta} \rightarrow \tilde{h}_{\alpha\beta} = h_{\alpha\beta} + \partial_\alpha\xi_\beta + \partial_\beta\xi_\alpha \\ \Rightarrow\ & h \rightarrow \tilde{h} = h + 2\eta^{\mu\nu}\partial_\mu\xi_\nu \end{aligned}$$

$$\Rightarrow \quad \bar{h}_{\alpha\beta} = h_{\alpha\beta} - \frac{1}{2} h \eta_{\alpha\beta} \quad \rightarrow \quad \bar{\tilde{h}}_{\alpha\beta} = \tilde{h}_{\alpha\beta} - \frac{1}{2}\tilde{h}\eta_{\alpha\beta} = \bar{h}_{\alpha\beta} + \partial_\alpha \xi_\beta + \partial_\beta \xi_\alpha - \partial^\mu \xi_\mu \eta_{\alpha\beta}$$

$$\Rightarrow \quad \partial^\nu \bar{h}_{\mu\nu} \quad \rightarrow \quad \partial^\nu \bar{\tilde{h}}_{\mu\nu} = \partial^\nu \Big[\bar{h}_{\mu\nu} + \underline{\partial_\mu \xi_\nu} + \partial_\nu \xi_\mu \underline{- \partial^\rho \xi_\rho \eta_{\mu\nu}} \Big] = \partial^\nu \bar{h}_{\mu\nu} + \partial^\nu \partial_\nu \xi_\mu \, . \tag{B.13}$$

Note that we have lowered the index of ∂^ν with the background metric $\eta_{\mu\nu}$ here. Next, we choose ξ_μ such that

$$\partial^\rho \partial_\rho \xi_\mu = -\partial^\rho \bar{h}_{\mu\rho} \, . \tag{B.14}$$

This is always possible by virtue of the existence and uniqueness of solutions to the wave equation. With this choice, we obtain the crucial transformation

$$\boxed{\partial^\nu \bar{h}_{\mu\nu} \quad \rightarrow \quad \partial^\nu \bar{\tilde{h}}_{\mu\nu} = \partial^\nu \bar{h}_{\mu\nu} + \partial^\nu \partial_\nu \xi_\mu \overset{!}{=} 0 \, ,} \tag{B.15}$$

which eliminates two terms in the linearized Einstein equation (B.10) and results in the linearized Einstein equations in the Lorenz gauge,

$$\boxed{\Box \bar{h}_{\mu\nu} = \partial^\rho \partial_\rho \bar{h}_{\mu\nu} = (-\partial_t^2 + \vec{\nabla}^2) \bar{h}_{\mu\nu} = -16\pi T_{\mu\nu} \, .} \tag{B.16}$$

B.2 Gravitational waves in the linear approximation

Gravitational waves are modulations in the fabric of spacetime that are generated by some strong-field source, say an inspiraling black-hole binary, and then propagate outwards. Far away from the source, their amplitude has diminished to such an extent that we can regard them as perturbations of the Minkowski metric. Furthermore, we treat the environment where the GWs travel as vacuum, so that in Lorenz gauge gravitational waves obey Eq. (B.16) with $T_{\mu\nu} = 0$ which is the flat-space wave equation

$$\Box \bar{h}_{\mu\nu} = (-\partial_t^2 + \vec{\nabla}^2) \bar{h}_{\mu\nu} = 0 \, . \tag{B.17}$$

Plane-wave solutions to this equation are readily obtained as

$$\bar{h}_{\mu\nu} = H_{\mu\nu} e^{\mathrm{i} k_\rho x^\rho} \, , \qquad H_{\mu\nu} = \mathrm{const} \, , \tag{B.18}$$

where k_ρ denotes the 4-wave vector. This solution has the following properties.

(1) Plugging the expression (B.18) into the linearized vacuum equations (B.17), we obtain $k^\rho k_\rho = 0$, i.e. the wave vector is a null vector and GWs propagate at the speed of light.

(2) The Lorenz gauge condition $\partial^\nu \bar{h}_{\mu\nu} = 0$ implies $k^\mu H_{\mu\nu} = 0$, so in this gauge, the waves are transverse to the direction of propagation. For a plane wave traveling in the z direction, for example, we have $k_\mu = \omega(-1, 0, 0, 1)$ and, hence, $H_{\mu 0} + H_{\mu 3} = 0$.

We can further simplify the expression for the plane wave by using the remaining gauge freedom. Indeed, Lorenz gauge is not unique, since the transformation (B.11) with

$$\xi_\mu = X_\mu e^{\mathrm{i}k_\rho x^\rho} \qquad \Rightarrow \qquad \partial^\nu \partial_\nu \xi_\mu = 0\,, \tag{B.19}$$

leaves the Lorenz gauge condition (B.14) unaltered. One can show that there exists a choice for the X_μ such that

$$H_{0\mu} = 0\,, \qquad H^\mu{}_\mu = 0\,. \tag{B.20}$$

This specific gauge is commonly referred to as *transverse-traceless* or TT for short. In this gauge, the plane-wave solution has the following additional properties.

(1) $h = 0 \quad \Rightarrow \quad \bar{h}_{\mu\nu} = h_{\mu\nu}$, so that the trace-reversed perturbation is equal to the original metric perturbation.

(2) For a plane wave propagating in the z direction, we have $H_{0\mu} = H_{3\mu} = H^\mu{}_\mu = 0$, so that

$$H_{\mu\nu} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & H_+ & H_\times & 0 \\ 0 & H_\times & -H_+ & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{B.21}$$

In order to see what effect such a GW has on an arrangement of test particles, we solve the geodesic equation for the metric $g_{\mu\nu} = \eta_{\mu\nu} + h_{\mu\nu}$ with the perturbation given by Eqs. (B.18), (B.21). Consider for this purpose a particle initially at rest in a background inertial frame, i.e. with four-velocity $u^\alpha = (1,\, 0,\, 0,\, 0)$. The geodesic equation at the initial time is given by

$$\frac{\mathrm{d}}{\mathrm{d}\tau} u^\alpha + \Gamma^\alpha_{\mu\nu} u^\mu u^\nu = \dot{u}^\alpha + \Gamma^\alpha_{00} = 0\,. \tag{B.22}$$

The Christoffel symbols are obtained from Eq. (B.5) and become

$$\Gamma^\alpha_{00} = \frac{1}{2}\eta^{\alpha\mu}(\partial_0 h_{\mu 0} + \partial_0 h_{0\mu} - \partial_\mu h_{00}) = 0 \qquad \text{since} \qquad H_{0\mu} = 0\,. \tag{B.23}$$

$u^\alpha = (1,\, 0,\, 0,\, 0)$ at all times is therefore the unique solution of the geodesic equation and the particle remains at fixed coordinate position x^μ as the GW passes through. Physical experiments, however, measure the proper distance that is obtained from

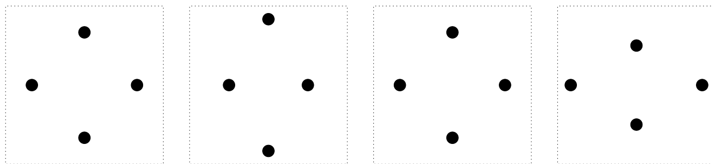
$$\mathrm{d}s^2 = -\mathrm{d}t^2 + (1 + h_+)\mathrm{d}x^2 + (1 - h_+)\mathrm{d}y^2 + 2h_\times \mathrm{d}x\,\mathrm{d}y + \mathrm{d}z^2\,, \tag{B.24}$$

where $\boxed{h_{+,\times} = H_{+,\times} e^{ik_\rho x^\rho}}$. We consider two cases.

Case 1: $H_\times = 0\,, \quad H_+ \neq 0$, so that h_+ oscillates. The proper distance between specific particles can be summarized as follows.

2 particles at $(-\delta,\ 0,\ 0)$, $(\delta,\ 0,\ 0)$ have $\mathrm{d}s^2 = (1 + h_+)4\delta^2$.

2 particles at $(0,\ -\delta,\ 0)$, $(0,\ \delta,\ 0)$ have $\mathrm{d}s^2 = (1 - h_+)4\delta^2$.

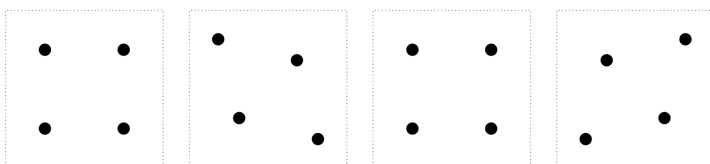


The figure illustrates the motion of the four test particles as the gravitational wave generates the oscillating perturbation h_+. This pattern motivates the index "+".

Case 2: $H_+ = 0\,,\quad H_\times \neq 0$, so that $h_\times$ oscillates. The proper distance between specific particles can be summarized as follows.

2 particles at $(-\delta,\ -\delta,\ 0)/\sqrt{2}$, $(\delta,\ \delta,\ 0)/\sqrt{2}$ have $\mathrm{d}s^2 = (1{+}h_\times)4\delta^2$.

2 particles at $(\delta,\ -\delta,\ 0)/\sqrt{2}$, $(-\delta,\ \delta,\ 0)/\sqrt{2}$ have $\mathrm{d}s^2 = (1{-}h_\times)4\delta^2$.



The figure illustrates the motion of the four test particles as the gravitational wave generates the oscillating perturbation $h_\times$. This pattern motivates the index "×".

B.3 Geodesic deviation

We can obtain the result (B.24) in an alternative way which turns out to be particularly useful for the comparison of the linearized equations with a fully non-linear treatment further below. This alternative derivation is based on the equation for geodesic deviation,

$$T^\mu \nabla_\mu (T^\nu \nabla_\nu S^\alpha) = R^\alpha{}_{\mu\rho\sigma} T^\mu T^\rho S^\sigma \qquad \Leftrightarrow \qquad \nabla_{\boldsymbol{T}} \nabla_{\boldsymbol{T}} \boldsymbol{S} = \boldsymbol{R}(\boldsymbol{T}, \boldsymbol{S})\boldsymbol{T}\,, \tag{B.25}$$

where S^α is the vector pointing from one geodesic to a nearby one and T^α is the tangent vector to the geodesic. This approach is frequently found in text books on general relativity, but care needs to be taken in interpreting this equation, in particular in the interpretation of the vector S^α. The geodesic deviation equation is manifestly covariant, and its interpretation requires us to relate the vector S^α to an observable. This is most conveniently achieved by choosing an appropriate frame or gauge. Our choice, however, is not the TT gauge but a local inertial or freely falling frame. In such a frame we can choose coordinates such that $g_{\mu\nu} = \eta_{\mu\nu} = \mathrm{diag}(-1,\ 1,\ 1,\ 1)$ and the first metric derivatives vanish, $\partial_\rho g_{\mu\nu} = 0$. This implies that the Levi-Civita connection also vanishes, $\Gamma^\alpha_{\beta\gamma} = 0$. Of course, we cannot gauge away spacetime curvature, so the second metric derivatives and the Riemann tensor will in general be non-zero.

Let us now consider the order in ϵ of terms in the geodesic deviation equation (B.25). On the right-hand side, the Riemann tensor is a first-order perturbation, so both sides of the equation must be $\mathcal{O}(\epsilon)$. On the left-hand side, the rate of change $\nabla_{\boldsymbol{T}}\nabla_{\boldsymbol{T}}\boldsymbol{S}$ is small even though $\boldsymbol{S}$ is of order unity. In words, $\boldsymbol{S}$ oscillates with an amplitude $\mathcal{O}(\epsilon)$ around its fixed initial magnitude of $\mathcal{O}(1)$. It is therefore sufficient to consider the tangent vector $\boldsymbol{T}$ at background order, which for particles initially at rest simply gives us the coordinate vector $\boldsymbol{T} = \boldsymbol{\partial}_t$, so that the geodesic deviation equation simplifies to

$$\partial_t^2 S^\alpha = R^\alpha{}_{00\sigma} S^\sigma \,. \tag{B.26}$$

This may appear like black magic; after all, we have gauged away the metric perturbations $h_{\mu\nu}$ out of the metric and the connection $\Gamma^\alpha_{\mu\nu}$ and readers may wonder how these perturbations can effect any physics. To answer this question, we have to return to the geodesic deviation equation (B.26) and, in particular, the Riemann tensor appearing on its right-hand side. The components of the Riemann tensor in the linearized formalism are given by Eq. (B.6) above and they are – that's the key point in this argument – gauge invariant, i.e. (Exercise) they are invariant under coordinate transformations of the type (B.11). We can therefore compute the Riemann tensor in the TT gauge and use them in the geodesic deviation equation in the local inertial frame. Using $h_{0\alpha} = 0$ in TT gauge as well as the standard symmetries of the Riemann tensor, we find

$$R_{000k} = 0\,, \qquad R_{j000} = 0\,, \qquad R_{j00k} = -R_{j0k0} = \frac{1}{2}\partial_0^2 h_{jk}\,, \tag{B.27}$$

where $j,\ k = 1,\ 2,\ 3$ are spatial indices. The components $R^\alpha{}_{00\sigma}$ are thus given by

$$\begin{aligned}
R^0{}_{00k} &= \eta^{0\mu} R_{\mu 00k} = -R_{000k} = 0\,,\\
R^j{}_{00k} &= \eta^{j\mu} R_{\mu 00k} = R_{j00k} = \frac{1}{2}\partial_0^2 h_{jk}\,,\\
R^0{}_{000} &= R^j{}_{000} = 0\,.
\end{aligned} \tag{B.28}$$

Assuming that the geodesic equation vector satisfies $S^0 = 0$ initially, we have $S^0 = 0$ always and can write the geodesic equation as

$$\begin{aligned}
&\partial_t^2 S^i = R^i{}_{00k} S^k = \frac{1}{2}\partial_t^2 h_{ik} S^k\,, \qquad h_{xx} = h_+ = -h_{yy}\,, \qquad h_{xy} = h_\times\\
\Rightarrow \qquad &\partial_t^2 S^x = \frac{1}{2}\left(\partial_t^2 h_{xx} S^x + \partial_t^2 h_{xy} S^y\right) = \frac{1}{2}\left(\partial_t^2 h_+ S^x + \partial_t^2 h_\times S^y\right)\\
\wedge\ &\partial_t^2 S^y = \frac{1}{2}\left(\partial_t^2 h_{yx} S^x + \partial_t^2 h_{yy} S^y\right) = \frac{1}{2}\left(\partial_t^2 h_\times S^x - \partial_t^2 h_+ S^y\right)\,.
\end{aligned} \tag{B.29}$$

The latter two equations are often encountered in text books, but it can easily lead to misconceptions. Even though they contain the metric perturbations h_+ and $h_\times$ of the TT gauge, they actually hold in the local inertial frame. More details about the potential confusion of analyzing GWs in linearized theory using different frames can be found in Leclerc's article [17].

Let us now consider the vector $\boldsymbol{S}$ with $S^0 = S^z = 0$ and

$$\begin{aligned} S^x &= \mathrm{d}x + \frac{1}{2}h_+\mathrm{d}x + \frac{1}{2}h_\times\mathrm{d}y\,, \\ S^y &= \mathrm{d}y + \frac{1}{2}h_\times\mathrm{d}x - \frac{1}{2}h_+\mathrm{d}y\,. \end{aligned} \tag{B.30}$$

Its second time derivatives are

$$\begin{aligned} \partial_t^2 S^x &= \frac{1}{2}\left(\partial_t^2 h_+\mathrm{d}x + \partial_t^2 h_\times\mathrm{d}y\right) = \frac{1}{2}\left(\partial_t^2 h_+ S^x + \partial_t^2 h_\times S^y\right) + \mathcal{O}(h_{+,\times}^2)\,, \\ \partial_t^2 S^y &= \frac{1}{2}\left(\partial_t^2 h_\times\mathrm{d}x - \partial_t^2 h_+\mathrm{d}y\right) = \frac{1}{2}\left(\partial_t^2 h_\times S^x - \partial_t^2 h_+ S^y\right) + \mathcal{O}(h_{+,\times}^2)\,, \end{aligned} \tag{B.31}$$

and we see that our S^α solves the geodesic deviation equation (B.29). Furthermore, its norm evaluated in the local inertial frame is

$$\begin{aligned} g_{\mu\nu}S^\mu S^\nu &= \eta_{\mu\nu}S^\mu S^\nu = (S^x)^2 + (S^y)^2 \\ &= \mathrm{d}x^2\left(1 + h_+ + h_\times\frac{\mathrm{d}y}{\mathrm{d}x}\right) + \mathrm{d}y^2\left(1 + h_\times\frac{\mathrm{d}x}{\mathrm{d}y} - h_+\right) + \mathcal{O}(h_{+,\times}^2) \\ &= \mathrm{d}x^2(1+h_+) + \mathrm{d}y^2(1-h_+) + 2h_\times\mathrm{d}y\mathrm{d}x + \mathcal{O}(h_{+,\times}^2)\,, \end{aligned} \tag{B.32}$$

which, at linear order, is exactly the proper separation we calculated above in Eq. (B.24) for particles with $\mathrm{d}t = \mathrm{d}z = 0$. The key benefit of computing this result from geodesic deviation is that it will allow us to compare the gauge invariant components of the Riemann tensor with the asymptotic expansion of the characteristic formalism in Sec. E without having to worry about how to transform into TT coordinates.

According to linearized theory, GWs therefore have two polarization modes and manifest themselves through a change in proper separation of test particles. This is indeed correct and is exactly the way the current network of ground-based detector measures GW events, including the first ever detection GW150914 [11]. It should be noted, however, that the nature of GWs remained under constant debate for about 40 years, including Einstein himself who vacillated on the issue. It was only around 1960 that results by Bondi, Pirani, Sachs and others demonstrated convincingly that gravitational waves are not merely a gauge effect but carry physical energy and are also predicted by the fully non-linear theory of general relativity. Understanding how this can be demonstrated is the main goal of the following sections. For this purpose, we need to take one step back and first discuss some fundamental properties of partial differential equations.

C Classification of Partial Differential Equations

Many physical systems are modelled in terms of partial differential equations (PDEs). Given the enormous number and range of physical systems, this provides us with a gargantuan zoo of differential equations and a correspondingly sizeable challenge to develop a toolbox for their solution. Quite remarkably, however, this zoo of equations exhibits a considerable degree of structure and most (relevant) PDEs can be classified into three groups that are referred to as *hyperbolic*, *parabolic* and *elliptic* PDEs. This classification is related to the propagation of information and the degree to which boundary or initial data determine a solution. These properties play a key role in the understanding of Einstein's equations of general relativity and we therefore start our discussion with a review of this classification of differential equations. One could easily spend an entire lecture series on this topic and readers are asked for forgiveness if in places we dispense with mathematical rigour and also refrain from a comprehensive treatment. At the same time, we attempt to go beyond the rather cavalier treatment that explains the categories by merely giving examples; statements such as "the wave equation is hyperbolic" or "the Laplace equation is elliptic" are absolutely correct, but little more descriptive than defining a star by saying "the sun is a star". Readers interested in more details of the structure of PDEs will find this in abundance in the still gold-standard book of Courant and Hilbert [18].

C.1 Second order PDEs of a single function

We start our discussion with second-order PDEs in a single variable. In this context, the term "order" refers to the degree of the highest derivative present in the equation. Most systems in contemporary physics are indeed governed by second-order PDEs, as for example the Maxwell equations of electrodynamics, the Schroedinger equation, the heat transport equation and Einstein's field equations of general relativity. The seeming absence of higher-order derivatives in the PDEs of physics may be related to the Ostrogradsky instability. Formally, Ostrogradsky's theorem states that a non-degenerate Lagrangian dependent on time derivatives higher than first corresponds to a Hamiltonian unbounded from below. While this does not entirely rule out theories involving higher-order derivatives, it severely restricts the construction of such theories [19]. We do not have to worry unduly about the consequences of Ostrogradsky's instability, but we note in passing that the study of higher-order theories is an important field of contemporary research and also plays an important role in attempts to modify Einstein's general relativity [20]. Finally, we note that we can reduce the order of derivatives in differential equations at the expanse of introducing auxiliary variables as in the trivial example

$$\partial_x^2 f = 0 \qquad \Leftrightarrow \qquad \partial_x f = g \quad \wedge \quad \partial_x g = 0\,. \tag{C.1}$$

This is a rather common approach, especially in the modeling of fluids using conservation laws [21]. For the time being, however, we dispense with this type of shenanigans and consider second-order PDEs plain and simple.

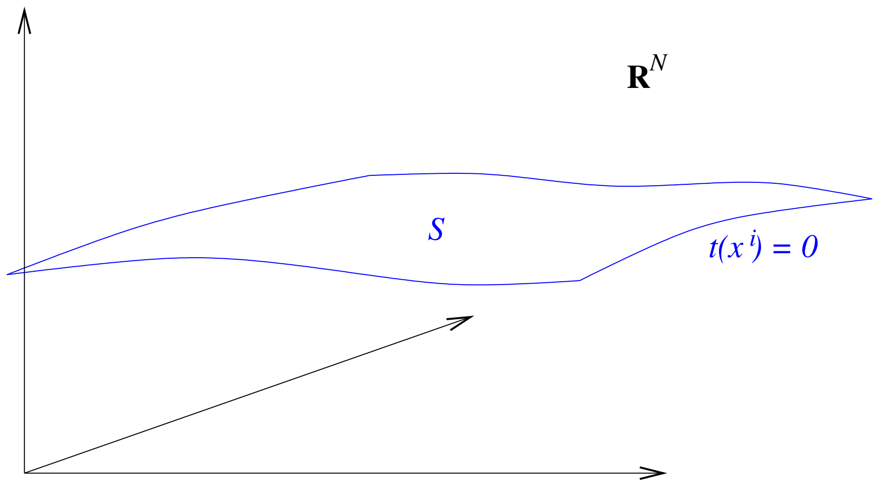


Figure 1: A level surface S defined by $t(x^i) = 0$ in the $\mathbb{R}^N$.

C.1.1 Classification of second-order linear PDEs

Def. : Let $x_i \in \mathbb{R}^N$, $f : \Omega \subset \mathbb{R}^N \to \mathbb{R}$. The *general partial differential equation of second order* is

$$F(x_i, f, \partial_i f, \partial_i \partial_j f) = 0\,, \tag{C.2}$$

where F is a sufficiently regular function in its $(N+1)^2$ arguments.

A *linear second-order partial differential equation* is an equation of the form

$$A_{mn}(x_i)\partial_m \partial_n f + b_m(x_i)\partial_m f + c(x_i) f + d(x_i) = 0\,. \tag{C.3}$$

Since partial derivatives commute, we can assume without loss of generality that the matrix A_{mn} is symmetric: $A_{mn} = A_{nm}$.

The *main* or *principal part* of the PDE is the set of terms that contain the highest derivatives. For example, the principal part of Eq. (C.3) is $A_{mn}\partial_m \partial_n f$.

Let us now consider a function $t(x_i)$ with non-zero gradient, $\nabla t \coloneqq (\partial_1 t, \ldots, \partial_N t) \neq 0$ everywhere and let S be the level surface defined by $t(x_i) = 0$ as shown in Fig. 1. Let us further assume that f and $\partial_i f$ are specified on S (or, to be more precise on the intersection of S with the domain Ω). The question we now wish to answer is whether, for the given PDE (C.3) and surface S, we can calculate all derivatives of the function f on S. If the answer is yes, then the solution f is determined away from S at least in the neighbourhood where the Taylor expansion of f converges.

In order to answer this question, we define a mapping $x^i \to \xi^a$, where i, $a = 1, \ldots, N$, on Ω given by

$$\xi_a = \xi_a(x_i) \qquad \text{for } a = 1, \ldots, N-1\,,$$

$$\xi_N = t(x_i)\,. \tag{C.4}$$

In words, we have chosen a new coordinate system such that our surface S is the level surface of one of our new coordinates, namely $\xi_N = t = 0$. With our earlier assumption $\nabla t \neq 0$, one can show that such a mapping with smooth functions ξ_a exist, at least in some neighbourhood of S. We can now regard $f(x_i) = f\big(x_i(\xi_a)\big)$ as a function of the new coordinates and obtain by chain rule

$$\begin{aligned} \partial_i f &:= \frac{\partial f}{\partial x_i} = \frac{\partial \xi_a}{\partial x_i}\frac{\partial f}{\partial \xi_a} =: \frac{\partial \xi_a}{\partial x_i}\partial_a f\,, \\ \partial_i\partial_j f &= \frac{\partial \xi_a}{\partial x_i}\partial_a\left(\frac{\partial \xi_b}{\partial x_j}\partial_b f\right) = \frac{\partial^2 \xi_b}{\partial x_i\,\partial x_j}\partial_b f + \frac{\partial \xi^a}{\partial x^i}\,\frac{\partial \xi^b}{\partial x^j}\partial_a\partial_b f\,. \end{aligned} \tag{C.5}$$

Our PDE (C.3) expressed in the new coordinate system is then given by

$$A_{mn}\frac{\partial \xi_a}{\partial x_m}\,\frac{\partial \xi_b}{\partial x_n}\partial_a\partial_b f + \text{lower order terms} = 0\,, \tag{C.6}$$

where the "lower order terms" involve at most first derivatives of f. Next, we recall that we have "initial" data on S for f and all $\partial_i f$ which we can directly translate into the new coordinates,

$$\begin{aligned} f(\xi_a) &= f(\xi_1,\,\ldots,\,\xi_{N-1},\,0) = f\big(\xi_a(x_i)\big)\,, \\ \partial_a f(\xi_a) &= \partial_a f(\xi_1,\,\ldots,\,\xi_{N-1},\,0) = \frac{\partial x_m}{\partial \xi_a}\,\left.\frac{\partial f}{\partial x_m}\right|_S\,. \end{aligned} \tag{C.7}$$

These initial data determine most of the second derivatives through direct evaluation of the differential quotients

$$\partial_b\partial_a f(\xi_1,\,\ldots,\,\xi_{N-1},\,0) = \lim_{h\to 0}\frac{\partial_a f(\xi_1,\,\ldots,\,\xi_b+h,\,\ldots,\,\xi_{N-1},\,0) - \partial_a f(\xi_1,\,\ldots,\,\xi_{N-1},\,0)}{h}\,, \tag{C.8}$$

for $b = 1,\,\ldots,\,N-1$. For $b = N$, however, this does not work, since we do not know f and $\partial_a f$ away from the surface S. Still, we can use Eq. (C.8) to formally substitute in Eq. (C.6) for all second derivatives except for $\partial^2 f/\partial\xi_N^2$, and our PDE can be written as

$$A_{mn}\frac{\partial \xi_N}{\partial x_m}\,\frac{\partial \xi_N}{\partial x_n}\,\frac{\partial^2 f}{\partial(\xi_N)^2} = \text{terms known on } S\,, \tag{C.9}$$

where on the left-hand side we sum over m and n, but *not* over N. We are therefore able to calculate the missing second derivative using the differential equation *if and only if*

$$A_{mn}\frac{\partial \xi_N}{\partial x_m}\,\frac{\partial \xi_N}{\partial x_n} \neq 0\,. \tag{C.10}$$

If this condition is satisfied, we can repeat the game by differentiating the PDE to compute all third derivatives and then all fourth derivatives and so forth. Recalling that $\xi_N = t$, the condition (C.10) motivates the important definition:

Def. : The differential equation

$$A_{mn}(x_i)\partial_m t\,\partial_n t = 0\,, \tag{C.11}$$

is called the *characteristic differential equation associated with the second-order, linear PDE* (C.3).

If $t(x_i)$ with $\nabla t \neq 0$ is a solution of (C.11), the surface defined by $t(x_i) = 0$ is called a *characteristic surface*.

In the special case that the matrix $A_{mn}(x_i)$ is positive or negative definite on Ω, then for any $t(x_i)$ with $\nabla t \neq 0$, we have

$$A_{mn}\partial_m t\,\partial_n t > 0 \qquad \text{or} \qquad A_{mn}\partial_m t\,\partial_n t < 0\,, \tag{C.12}$$

so that Eq. (C.10) is satisfied and the PDE admits no characteristic surface. More generally, second-order linear PDEs are classified as follows.

Def. : The PDE

$$A_{mn}(x_i)\partial_m f\,\partial_n f + b_m(x_i)\partial_m f + c(x_i)f + d(x_i) = 0\,, \tag{C.13}$$

is said to be of type (α, β, γ) at $x_i \in \Omega$ if α Eigenvalues of $A_{mn}(x_i)$ are positive, β Eigenvalues are negative and γ Eigenvalues are 0 with $\alpha + \beta + \gamma = N$.

The PDE is:

- *elliptic* if it is of type $(N,\,0,\,0)$ or $(0\,,N\,,0)$, i.e. if all Eigenvalues are non-zero and have the same sign.
- *parabolic* if it is of type $(N-1,\,0,\,1)$ or $(0,\,N-1,\,1)$, i.e. if one Eigenvalue is zero and all others are non-zero and have the same sign.
- *hyperbolic* if it is of type $(N-1,\,1,\,0)$ or $(1,\,N-1,\,0)$, i.e. all Eigenvalues are non-zero and exactly one of them has the opposite sign of all the others.

A few remarks are in order.

1. Note that in the parabolic and hyperbolic case, we can always find a non-trivial (i.e. non-vanishing) linear combination V_m of Eigenvectors such that[2] $A_{mn}V_mV_n = 0$, i.e. at every point x_i there exists a non-zero $\partial_m t$ that satisfies the characteristic differential equation (C.11) and therefore the PDE admits a characteristic surface. In the elliptic case, in contrast, A_{mn} is positive or negative definite, the only solution to the characteristic equation is the null vector and we cannot construct a characteristic surface.

[2]The key point is that we can expand V_m in an orthonormal Eigenvector basis (since A_{mn} is symmetric). Then $A_{mn}V_mV_n$ becomes a sum of terms $\propto \lambda_i \boldsymbol{W}^{(i)} \cdot \boldsymbol{W}^{(i)}$, where $\boldsymbol{W}^{(i)}$ is the ith Eigenvector and λ_i the ith Eigenvalue. Since $\boldsymbol{W}^{(i)} \cdot \boldsymbol{W}^{(j)} = \delta_{ij}$, this simply becomes a weighted sum of the Eigenvalues; for appropriate weights, i.e. an appropriate $\boldsymbol{V}$, this sum can vanish because one Eigenvalue differs in sign from the others.

2. According to this definition, there are other types of PDEs aside from elliptic, parabolic and hyperbolic. But we do not concern ourselves with these; they play no role in the physics we are interested in (nor in any other physics for all I am aware of).
3. The type of a PDE depends on the point x^i and may change across the domain Ω.

Examples

(1) The Tricomi equation

$$y\partial_x^2 f + \partial_y^2 f = 0\,, \tag{C.14}$$

appears in the theory of transsonic flow. The matrix of its principal part is

$$A^{mn} = \begin{pmatrix} y & 0 \\ 0 & 1 \end{pmatrix} \tag{C.15}$$

Clearly, the Eigenvalues are y and 1, so the Tricomi equation is elliptic for $y > 0$, parabolic on $y = 0$ and hyperbolic for $y < 0$.

(2) The Laplace equation in 3 dimensions is

$$\triangle f \coloneqq \partial_x^2 f + \partial_y^2 f + \partial_z^2 f = 0\,, \tag{C.16}$$

with $A^{mn} = \delta^{mn}$ and all 3 Eigenvalues are 1. The Laplace equation is therefore elliptic everywhere. For any surface S given by $t(x^i) = 0$, $\nabla t \neq 0$, we can compute all derivatives of f on S provided we have initial data f, $\partial_i f$ on S. The solution is thus fully determined by the initial data at least in some neighbourhood of S.

(3) The wave equation in 3+1 dimensions,

$$\Box f \coloneqq -\partial_t^2 f + \partial_x^2 f + \partial_y^2 f + \partial_z^2 f = 0\,, \tag{C.17}$$

is hyperbolic everywhere with Eigenvalues -1, 1, 1 and 1.

(4) The heat equation in 3+1 dimensions

$$-\partial_t f + \partial_x^2 f + \partial_y^2 f + \partial_z^2 f = 0\,, \tag{C.18}$$

is parabolic, since one Eigenvalue is 0 and the three others are 1.

C.1.2 Principal axes*

Let us briefly recapitulate some key properties of matrices and their eigenvalue decomposition.

<u>**Def. :**</u> Let $\boldsymbol{A}$ be a $N \times N$ matrix. $\boldsymbol{V} \in \mathbb{R}^N$ is an *Eigenvector* with *Eigenvalue* λ of $\boldsymbol{A}$ if

$$\boldsymbol{AV} = \lambda \boldsymbol{V} \qquad \text{or} \qquad A_{mn}V_n = \lambda V_m\,. \tag{C.19}$$

Symmetric matrices have particularly convenient Eigenvalues and Eigenvectors.

Proposition: A symmetric $N \times N$ matrix $A_{ij} = A_{ji}$ has n real Eigenvalues and the associated Eigenvectors can be chosen such that they form a set of N mutually orthonormal vectors.

The proof can be found in most standard textbooks on linear algebra. We next arrange the N Eigenvectors as column vectors of the new $N \times N$ matrix $\mathbf{Q}$,

$$\mathbf{Q} = \begin{pmatrix} Q_{11} & Q_{12} & \dots & Q_{1N} \\ Q_{21} & Q_{22} & \dots & Q_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ Q_{N1} & Q_{N2} & \dots & Q_{NN} \end{pmatrix} \tag{C.20}$$

$$= V_{k(2)}\,,$$

where we denote by $V_{k(2)}$ the components of the second Eigenvector $\boldsymbol{V}_{(2)}$. The matrix $\mathbf{Q}$ is orthogonal in its columns by construction since the Eigenvectors are orthonormal,

$$\delta_{ij} = V_{m(i)} V_{m(j)} = Q_{mi} Q_{mj} = Q^{\intercal}_{im} Q_{mj}\,. \tag{C.21}$$

In index free notation, this gives us

$$\mathbf{Q}^{\intercal}\mathbf{Q} = \boldsymbol{I} \quad\Rightarrow\quad \mathbf{Q}^{-1} = \mathbf{Q}^{\intercal} \quad\Rightarrow\quad \mathbf{Q}\mathbf{Q}^{\intercal} = \mathbf{Q}\mathbf{Q}^{-1} = \boldsymbol{I} \quad\Rightarrow\quad Q_{im} Q_{jm} = \delta_{ij}\,, \tag{C.22}$$

so the rows of $\mathbf{Q}$ are also orthonormal. If we denote by $\lambda_{(i)}$ the i-th Eigenvalue, we have N Eigenvalue equations (no summation over i)

$$\begin{aligned} & A_{km} V_{m(i)} = \lambda_{(i)} V_{k(i)} && \Big|\ V_{k(j)}\,\cdot \\ \Rightarrow\quad & V_{k(j)} A_{km} V_{m(i)} = \lambda_{(i)} V_{k(j)} V_{k(i)} = \lambda_{(i)} \delta_{(i)(j)} \\ \Rightarrow\quad & Q_{kj} A_{km} Q_{mi} = \lambda_{(i)} \delta_{ij} \\ \Rightarrow\quad & \mathbf{Q}^{\intercal}\mathbf{A}\mathbf{Q} = \begin{pmatrix} \lambda_{(1)} & 0 & \cdots & 0 \\ 0 & \lambda_{(2)} & \cdots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \cdots & \lambda_{(N)} \end{pmatrix} =: \boldsymbol{\Lambda}\,. \end{aligned} \tag{C.23}$$

We have summarized this very familiar result in more detail here to clarify how the Eigendecomposition of a matrix looks like in index notation.

The Eigendecomposition is of particular convenience for second order PDEs where the principal part has constant coefficients, i.e. Eq. (C.3) with $A_{mn} = \text{const}$. As mentioned earlier, we can assume a symmetric A_{mn} without loss of generality and therefore apply the above Eigendecomposition. More specifically, we consider the Eigenvectors $\boldsymbol{V}_{(k)}$ of the matrix A_{mn}

and let them constitute the columns of the orthogonal matrix $Q_{ik} := V_{i(k)}$. Next, we transform to a new coordinate system,

$$
\begin{aligned}
& y_i = Q_{mi} x_m \qquad \Rightarrow \qquad \frac{\partial y_i}{\partial x_j} = Q_{mi}\delta_{mj} = Q_{ji} \\
\Rightarrow \quad & \frac{\partial f}{\partial x_n} = \frac{\partial f}{\partial y_j}\frac{\partial y_j}{\partial x_n} = Q_{nj}\frac{\partial f}{\partial y_j} \\
\Rightarrow \quad & \frac{\partial^2 f}{\partial x_m \partial x_n} = Q_{mi}Q_{nj}\frac{\partial^2 f}{\partial y_i \partial y_j} \\
\Rightarrow \quad & A_{mn}\frac{\partial^2 f}{\partial x_m \partial x_n} = A_{mn}Q_{mi}Q_{nj}\frac{\partial^2 f}{\partial y_i \partial y_j} = Q^{\intercal}_{im}A_{mn}Q_{nj}\frac{\partial^2 f}{\partial y_i \partial y_j} = \lambda_{(i)}\delta_{ij}\frac{\partial^2 f}{\partial y_i \partial y_j} \\
\Rightarrow \quad & A_{mn}\frac{\partial^2 f}{\partial x_m \partial x_n} = \lambda_{(i)}\frac{\partial^2 f}{\partial y_i\, \partial y_i} = \lambda_{(i)}\frac{\partial^2 f}{\partial y_i^2} \qquad \text{(summation over } i\,!) \,.
\end{aligned} \tag{C.24}
$$

This procedure allows us to eliminate all mixed derivatives and essentially, we can reduce physically relevant second-order linear PDEs with constant coefficients into a form whose principal part very much resembles that of the wave, heat or Laplace equation.

C.1.3 Second-order PDEs in 2 dimensions

Two-dimensional domains are particularly easy to visualize and draw on sheets of paper. We therefore analyze in this section PDEs on domains $\Omega \subset \mathbb{R}^2$.

C.1.3.1 Classification of PDEs in 2 dimensions

We now consider linear, second-order PDEs in two independent variables,

$$
a(x,y)\partial_x^2 f + 2b(x,y)\partial_x\partial_y f + c(x,y)\partial_y^2 f + \text{lower-order terms} = 0\,, \tag{C.25}
$$

on some domain $\Omega \subset \mathbb{R}^2$. The characteristic differential equation associated with (C.25) is

$$
a(\partial_x t)^2 + 2b\partial_x t\,\partial_y t + c(\partial_y t)^2 = 0\,. \tag{C.26}
$$

Let us assume that we have a solution to this characteristic equation given by $t(x,y)$ with $\nabla t \neq 0$ on Ω. We next consider the level sets of $t(x,y)$ given by

$$
\Big\{(x,y) \;\Big|\; t(x,y) = \text{const}\Big\}\,.
$$

In 2 dimensions the level sets are, of course, curves. At a given point $(x_0, y_0) \in \Omega$ we can assume without loss of generality that $\partial_y t \neq 0$; otherwise we would inevitably have $\partial_x t \neq 0$ and could

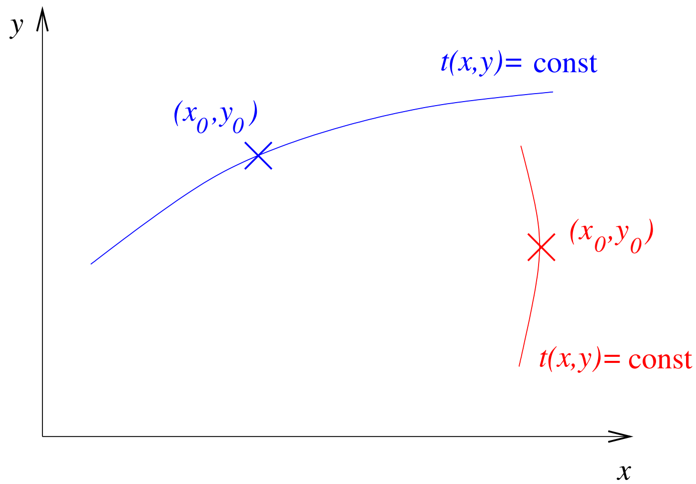


Figure 2: Two examples for a level set (curve) $t(x,y) = \text{const}$ in the $\mathbb{R}^2$. In the (upper) blue example, we have a curve where at (x_0, y_0), the derivative $\partial_y t \neq 0$. In the (lower) red example, we have $\partial_y t = 0$ at (x_0, y_0); the level curve is vertical (parallel to the y axis) at this point.

simply swap the coordinate labels. Since $\partial_y t \neq 0$, the curve $t(x,y) = \text{const}$ will not be parallel to the y axis in some neighbourhood of (x_0, y_0); cf. Fig. 2. In that case, we can represent the curve $t(x,y) = \text{const}$ in the form $y(x)$ in some neighbourhood of (x_0, y_0). If we parametrize the curve with $\lambda \in \mathbb{R}$, we have $t(\lambda) = t\big(x(\lambda), y(\lambda)\big) = \text{const}$ and, hence,

$$\frac{\mathrm{d}t}{\mathrm{d}\lambda} = \frac{\partial t}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}\lambda} + \frac{\partial t}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}\lambda} = 0$$

$$\Rightarrow \quad \frac{\mathrm{d}y}{\mathrm{d}x} = \frac{\mathrm{d}y}{\mathrm{d}\lambda}\left(\frac{\mathrm{d}x}{\mathrm{d}\lambda}\right)^{-1} = -\frac{\partial_x t}{\partial_y t}\,. \tag{C.27}$$

This allows us to write the characteristic equation (C.26) as

$$a\left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)^2 - 2b\frac{\mathrm{d}y}{\mathrm{d}x} + c = 0\,. \tag{C.28}$$

Provided $a \neq 0$, we can solve this equation for $y' := \frac{\mathrm{d}y}{\mathrm{d}x}$,

$$(y')^2 - \frac{2b}{a}y' + \frac{c}{a} = 0 \qquad \Rightarrow \qquad y' = \frac{b}{a} \pm \sqrt{\frac{b^2}{a^2} - \frac{c}{a}} = \frac{1}{a}\left(b \pm \sqrt{b^2 - ac}\right)\,. \tag{C.29}$$

Real solutions only exist if $b^2 \geq ac$ whereas characteristic surfaces do not exist if $b < ac$. We can indeed confirm this result with our general classification of PDEs from the definition (C.13). For this purpose, we compute the Eigenvalues of $\begin{pmatrix} a & b \\ b & c \end{pmatrix}$,

$$\begin{vmatrix} a-\lambda & b \\ b & c-\lambda \end{vmatrix} = ac - (a+c)\lambda + \lambda^2 - b^2 = 0$$

$$\Rightarrow \quad \lambda^2 - (a+c)\lambda - (b^2 - ac) = 0$$

$$\Rightarrow \quad \lambda_\pm = \frac{a+c}{2} \pm \sqrt{\frac{(a+c)^2}{4} + (b^2 - ac)} = \frac{a+c}{2}\left[1 \pm \sqrt{1 + 4\frac{b^2 - ac}{(a+c)^2}}\,\right] \tag{C.30}$$

As expected for a symmetric matrix, the Eigenvalues are always real,

$$1 + 4\frac{b^2 - ac}{(a+c)^2} = \frac{1}{(a+c)^2}\left[(a+c)^2 + 4b^2 - 4ac\right] = \frac{(a-c)^2 + 4b^2}{(a+c)^2} \geq 0\,. \tag{C.31}$$

Next, we see that the two Eigenvalues $\lambda_\pm$ have the same sign if $b^2 < ac$, and opposite signs if $b^2 > ac$, and one Eigenvalue vanishes if $b^2 = ac$. Finally, this analysis also covers the case $a = 0$ which implies

$$\lambda_\pm = \frac{c}{2} \pm \sqrt{\frac{c^2}{4} + b^2}\,. \tag{C.32}$$

Clearly, the Eigenvalues have opposite signs unless $b = 0$ in which case we obtain $\lambda_- = 0$. We can summarize this result for arbitrary a as follows: At a point $(x_0, y_0) \in \Omega$, the PDE (C.25) is

1. elliptic if $b^2 < ac$; $\lambda_\pm$ have the same sign.
2. hyperbolic if $b^2 > ac$; $\lambda_\pm$ have opposite signs.
3. parabolic if $b^2 = ac$; in that case, $\lambda_- = 0$.

C.1.3.2 The normal form of hyperbolic PDEs in 2 dimensions

Let us now consider a PDE that is hyperbolic in some neighbourhood of the point (x_0, y_0). Then we have two different solutions, which we denote by $u(x,y)$ and $v(x,y)$, to the characteristic equation (C.26) with $\nabla u \neq 0 \neq \nabla v$. We can always rotate the coordinates (x,y) such that in a neighbourhood of (x_0, y_0) we have $\partial_y u \neq 0 \neq \partial_y v$. This allows us to write the curves of constant u and v, respectively, in the form

$$y = y_1(x) \qquad \text{along which } u = \text{const}\,,$$

$$y = y_2(x) \qquad \text{along which } v = \text{const}\,.$$

with

$$y_1'(x) = -\frac{\partial_x u}{\partial_y u}\,, \qquad y_2'(x) = -\frac{\partial_x v}{\partial_y v} \tag{C.33}$$

$$\Rightarrow \quad \partial_x u + y_1' \partial_y u = 0 \qquad \wedge \qquad \partial_x v + y_2' \partial_y v = 0\,. \tag{C.34}$$

We illustrate the corresponding level sets $u(x,y) = \text{const}$ and $v(x,y) = \text{const}$ in Fig. 3 and proceed by identifying some of their properties.

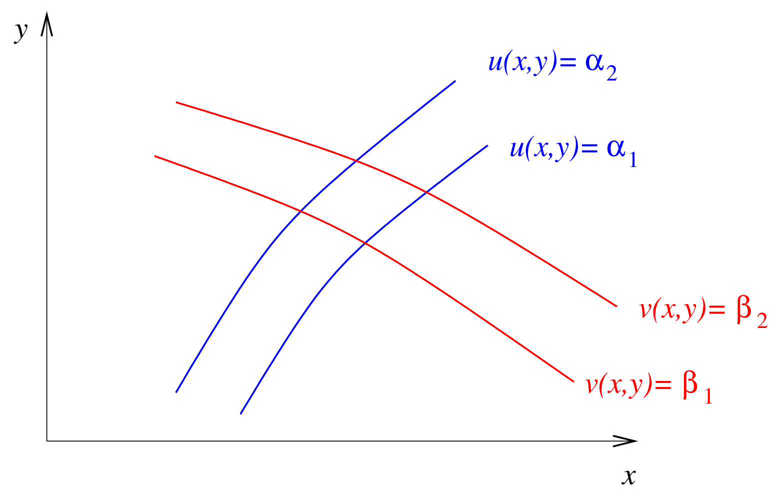


Figure 3: Two level sets of curves given by $u(x, y) = \text{const}$ and by $v(x, y) = \text{const}$.

Lemma : Let $u(x, y)$, $v(x, y)$ be two different solutions to the characteristic equation (C.26) associated with a second-order hyperbolic PDE of the type (C.25) with $\nabla u \neq 0 \neq \nabla v$. Then the two families of curves defined by $u = \text{const}$ and by $v = \text{const}$ satisfy the following:

(i) Curves from different families cannot touch, i.e. intersect each other *with* equal tangent direction.

(ii) The functions u and v obey the inequality

$$\partial_x u \, \partial_y v - \partial_y u \, \partial_x v \neq 0 \, .$$

Proof.

(i) At points of intersection, curves belonging to the two different families have a slope given by Eq. (C.29). Since the two curves belong to different families, we have the + sign in Eq. (C.29) for one of them and the minus sign for the other. The difference between their slopes is therefore

$$y_2' - y_1' = \frac{1}{a}\left(b \pm \sqrt{b^2 - ac}\right) - \frac{1}{a}\left(b \mp \sqrt{b^2 - ac}\right) = \pm 2\frac{\sqrt{b^2 - ac}}{a} \neq 0 \tag{C.35}$$

since $b^2 > ac$ for a hyperbolic PDE.

(ii) Plugging Eq. (C.33) into $y_2' - y_1' \neq 0$ gives us

$$-\frac{\partial_x v}{\partial_y v} + \frac{\partial_x u}{\partial_y u} \neq 0 \qquad \Rightarrow \qquad \partial_x u \, \partial_y v - \partial_x v \, \partial_y u \neq 0 \, . \tag{C.36}$$

□

Def. : The solutions $u(x,y)$, $v(x,y)$ to the characteristic equation (C.26) associated with the PDE (C.25) are called *characteristic coordinates*.

Proposition: In characteristic coordinates, a hyperbolic PDE of the form (C.25) becomes

$$\partial_u \partial_v f = \text{lower order terms}\,. \tag{C.37}$$

Proof. Introducing the short-hand notation $u_x := \partial_x u$, $f_u := \partial_u f$, $f_{uv} = \partial_v \partial_u f$ etc., we find by chain rule that

$$\begin{aligned}
\partial_x &= \partial_x u\,\partial_u + \partial_x v\,\partial_v\,, \qquad\qquad \partial_y = \partial_y u\,\partial_u + \partial_y v\,\partial_v\,,\\
f_x &= u_x f_u + v_x f_v\,,\\
f_y &= u_y f_u + v_y f_v\,,\\
f_{xx} &= \partial_x(u_x f_u + v_x f_v) \;=\; u_{xx} f_u + u_x^2 f_{uu} + u_x v_x f_{vu} + v_{xx} f_v + v_x u_x f_{uv} + v_x^2 f_{vv}\\
&= u_x^2 f_{uu} + 2u_x v_x f_{uv} + v_x^2 f_{vv} + u_{xx} f_u + v_{xx} f_v\,,\\
f_{xy} &= (u_y \partial_u + v_y \partial_v)(u_x f_u + v_x f_v)\\
&= u_{xy} f_u + v_{xy} f_v + u_y u_x f_{uu} + (u_y v_x + u_x v_y) f_{uv} + v_x v_y f_{vv}\\
f_{yy} &= u_y^2 f_{uu} + 2u_y v_y f_{uv} + v_y^2 f_{vv} + u_{yy} f_u + v_{yy} f_v\,.
\end{aligned}$$

The principal part of our PDE thus becomes

$$a f_{xx} + 2b f_{xy} + c f_{yy} = \alpha f_{uu} + 2\beta f_{uv} + \gamma f_{vv}\,,$$

with

$$\begin{aligned}
\alpha &= a u_x^2 + 2b u_x u_y + c u_y^2 = 0\,,\\
2\beta &= a 2 u_x y_x + 2b(u_y v_x + v_y u_x) + c 2 u_y v_y\,,\\
\gamma &= a v_x^2 + 2b v_x v_y + c v_y^2 = 0\,,
\end{aligned}$$

where α and γ vanish since u and v satisfy the characteristic equation (C.26).

Furthermore, a lengthy but straightforward calculation (best performed with a program like `Mathematica` or `Maple`) shows that

$$\alpha\gamma - \beta^2 = (ac - b^2)(u_x v_y - u_y v_x)^2 \overset{!}{<} 0\,,$$

since for a hyperbolic PDE $b^2 > ac$. So $\beta^2 > 0$ and $\beta \neq 0$. ☐

Example

(1) Restoring the more common coordinate names (t, r) in place of the abstract (x, y), the wave equation for a free field in one spatial dimension is given by

$$\partial_t^2 f - \partial_r^2 f = 0\,, \tag{C.38}$$

and has the associated characteristic differential equation

$$\begin{aligned} & (\partial_t u)^2 - (\partial_r u)^2 = (\partial_t u + \partial_r u)(\partial_t u - \partial_r u) = 0 \\ \Rightarrow\quad & \partial_t u = -\partial_r u \qquad \vee \qquad \partial_t u = \partial_r u \\ \Rightarrow\quad & r_1'(t) = 1\,, \qquad\qquad r_2'(t) = -1\,. \end{aligned} \tag{C.39}$$

The solutions to the characteristic equation are therefore given by

$$u(t, r) = t - r\,, \qquad\qquad v(t, r) = t + r\,. \tag{C.40}$$

Transforming the wave equation (C.38) to characteristic coordinates gives us

$$\begin{aligned} & \partial_t = u_t\partial_u + v_t\partial_v = \partial_u + \partial_v \qquad \wedge \qquad \partial_r = u_r\partial_u + v_r\partial_v = -\partial_u + \partial_v \\ \Rightarrow\quad & 0 = \partial_t^2 f - \partial_r^2 f = (\partial_u + \partial_v)^2 f - (\partial_u - \partial_v)^2 f = 4\partial_u\partial_v f \\ \Rightarrow\quad & \partial_v\partial_u f = 0\,. \end{aligned} \tag{C.41}$$

Writing this as $\partial_v(\partial_u f) = 0$, we see that $\partial_u f$ is a function only of u, so for any C^2 function that satisfies the wave equation we have $\partial_u f = \phi(u)$ for some C^1 function ϕ. Integrating in u for given fixed v, we thus obtain

$$f(u, v) = \int \phi(u)\mathrm{d}u + G(v)\,, \tag{C.42}$$

where $G(v)$ acts as the v dependent integration constant. Denoting $F(u) \coloneqq \int \phi(u)\mathrm{d}u$, we obtain the general solution to the wave equation

$$f(u, v) = F(u) + G(v)\,. \tag{C.43}$$

On the other hand, every function of this form clearly satisfies $\partial_v\,\partial_u f = 0$. In summary, f solves the wave equation $\partial_t^2 f - \partial_r^2 f = 0$ if and only if

$$f(t, r) = F(t - r) + G(t + r)\,, \tag{C.44}$$

for some C^1 functions F, G.

Let us also use this example to illustrate the deficiency of specifying initial data on a characteristic surface (or curve in this two-dimensional example). Assume that we prescribe $f(u, 0) = f_0(u)$ on the characteristic curve $v = 0$ as illustrated in Fig. 4.

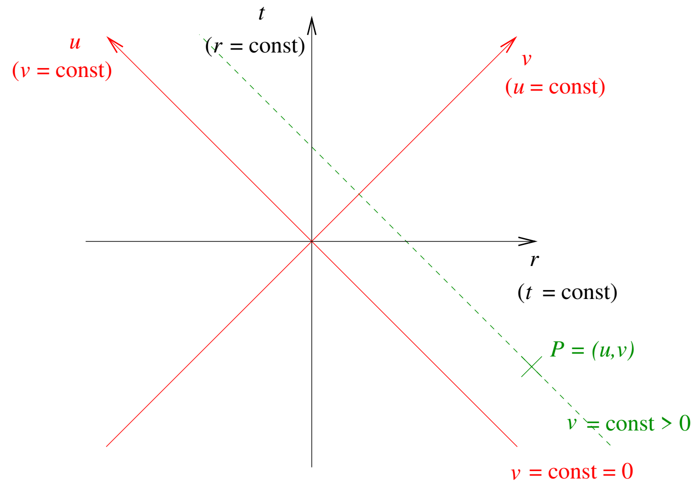


Figure 4: Characteristic coordinates $(u, v) = (t - r, t + r)$ for the wave equation $\partial_t^2 f - \partial_r^2 f = 0$ in one spatial dimension. If we specify initial data $f(u, 0) = f_0(u)$ at $v = 0$, we do not have enough information to determine the solution $f(u, v)$ at any $v \neq 0$, say at point P on the green dashed line.

That allows us to determine $\partial_u f$ on the slice $v = 0$. The differential equation then predicts $\partial_u f$ at least in some neighbourhood $v \neq 0$, for example on the green dashed curve in Fig. 4. However, we cannot reconstruct the solution f itself at any point on this dashed curve, since we do not know the integration constant $G(v)$. The problem would not arise if we had specified initial data on a non-characteristic surface, as for example on the horizontal curve $t = 0$.

We have seen in this example two special features of the characteristic surfaces. First, without some further information, initial data on a characteristic surface does not determine the solution even in a small neighbourhood of the surface. Second, characteristic coordinates significantly simplify the structure of the underlying PDE. A third feature may already become apparent from our physical insight into the wave equation. The characteristics in Fig. 4 represent the light cone of the wave equation and we know that information propagates along the light cones. In a sense that we will make more concrete further below, information propagates along characteristic curves.

C.2 *Systems of PDEs

So far, we have only considered single PDEs for one single function. We will now generalize these ideas to systems of PDEs. This is most conveniently achieved by considering first-order systems, i.e. the PDE only contains first derivatives. Second-order PDEs can always be converted into such a form by introducing auxiliary variables as we will see in some of our examples.

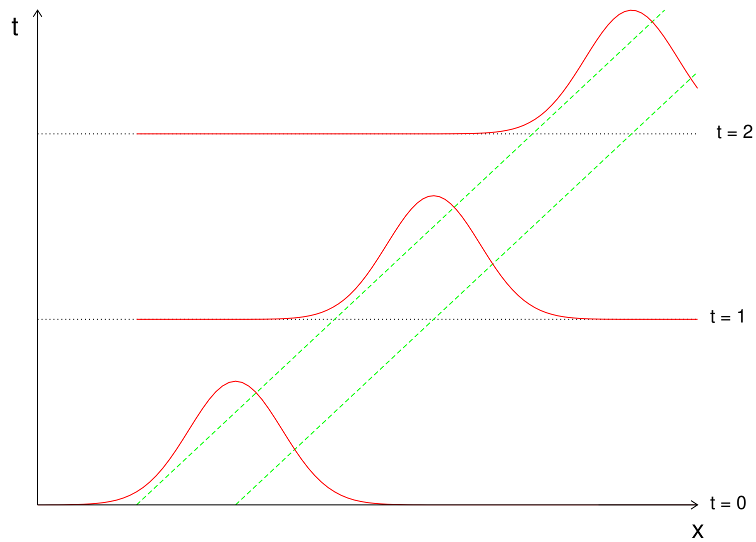


Figure 5: Illustration of a solution to the advection equation (C.45) in the (t, x) plane. Suppose we prescribe initial data $f(0, x)$ in the form of a Gaussian profile at $t = 0$. Along the (green dashed) curves $x = \lambda t + x_0$, the value of f remains constant according to Eq. (C.47). In consequence, the Gaussian pulse simply propagates to the right with velocity λ without otherwise changing its shape. Note that the (red) Gaussian curves are not to be regarded as curves in the (t, x) plane; if I could draw in $3D$, they would pop out of the paper instead.

C.2.1 *The advection equation

Before we explore more general first-order systems, we will illustrate some of their fundamental features in the case of the simplest possible PDE, the advection equation in one variable and two dimensions,

$$\partial_t f + \lambda \partial_x f = 0 \,, \qquad \lambda \in \mathbb{R} \,. \tag{C.45}$$

Let us now consider the curves

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \lambda \qquad \Rightarrow \qquad x(t) = \lambda t + x_0 \,. \tag{C.46}$$

Along these curves,

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial t} + \frac{\mathrm{d}x}{\mathrm{d}t}\frac{\partial f}{\partial x} = \frac{\partial f}{\partial t} + \lambda \frac{\partial f}{\partial x} = 0 \,, \tag{C.47}$$

by virtue of the PDE (C.45). Now suppose, we specify initial data in the form $f(0, x) = f_0(x)$, say a Gaussian profile as in Fig. 5. For every x_0, the solution f along the curve $x = \lambda t + x_0$ remains constant at its initial value $f(0, x_0)$. The Gaussian profile therefore simply propagates to the right with velocity λ but does not otherwise change its shape. We say, the Gaussian pulse is *advected* with velocity λ. As we will see later, the curves $x = \lambda t + x_0$ are actually the characteristic curves of the PDE (C.45). Note also the similarity to the propagation of light in relativity; for reasons that will become clear soon, the advection equation is sometimes also referred to as the *one-way wave equation*.

We can easily generalize the advection equation to varying propagation speeds $\lambda(t,x)$. In practice, such an x dependence appears most commonly in the form of *conservation laws*, i.e. PDEs of the form $\partial_t f + \partial_x F(f(t,x)) = 0$ where F is a *flux function* depending on the solution f. The generalization of Eq. (C.45) is therefore often written in the form

$$\begin{aligned} &\frac{\partial f}{\partial t} + \frac{\partial}{\partial x}\Big(\lambda(t,x) f\Big) = 0 \\ \Rightarrow \quad &\left(\frac{\partial}{\partial t} + \lambda(t,x)\frac{\partial}{\partial x}\right) f(t,x) = -\lambda'(t,x) f(t,x)\,, \end{aligned} \tag{C.48}$$

where $\lambda'(t,x) = \partial\lambda/\partial x$. As before, we consider the characteristic curves

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \lambda(t,x) \tag{C.49}$$

along which we can now construct a solution to Eq. (C.48) by solving for each x_0 the ordinary differential equation (ODE)

$$\frac{\mathrm{d}}{\mathrm{d}t} f\Big(x(t),t\Big) = -\lambda'(t,x) f(x,t)\,. \tag{C.50}$$

One can show that for initial data $f(0,x) = f_0(x) \in C^k(-\infty,\infty)$, the solution $f(t,x)$ is equally smooth in space and time, i.e. $f \in C^k((-\infty,\infty)\times(0,\infty))$.

C.2.2 *Burgers' equation

As a further extension of the advection equation, we may allow the propagation speed λ to depend on the solution f itself. This step has such dramatic consequences that we promote our discussion of this case to a separate subsection. Again, this type of equations often arises in conservation laws

$$\partial_t f + \partial_x F(f) = \partial_t f + F'(f)\partial_x f = 0\,. \tag{C.51}$$

First-order differential equations where the coefficients of the partial derivatives depend on the function f, but not on derivatives of f, are commonly referred to as *quasi-linear*; they are linear in the derivatives but not in the function f. The prototypical example for a scalar (i.e. one dependent variable) first-order quasi-linear PDE is Burgers' equation,

$$\partial_t f + \partial_x\left(\tfrac{1}{2}f^2\right) = \partial_t f + f\partial_x f = 0\,. \tag{C.52}$$

Comparing with Eq. (C.45), we see that this is an advection equation where the advection speed is equal to the function value. Along the curves

$$\frac{\mathrm{d}x}{\mathrm{d}t} = f\,, \tag{C.53}$$

we find

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial t} + \frac{\mathrm{d}x}{\mathrm{d}t}\frac{\partial f}{\partial x} = \frac{\partial f}{\partial t} + f\frac{\partial f}{\partial x} = 0\,, \tag{C.54}$$

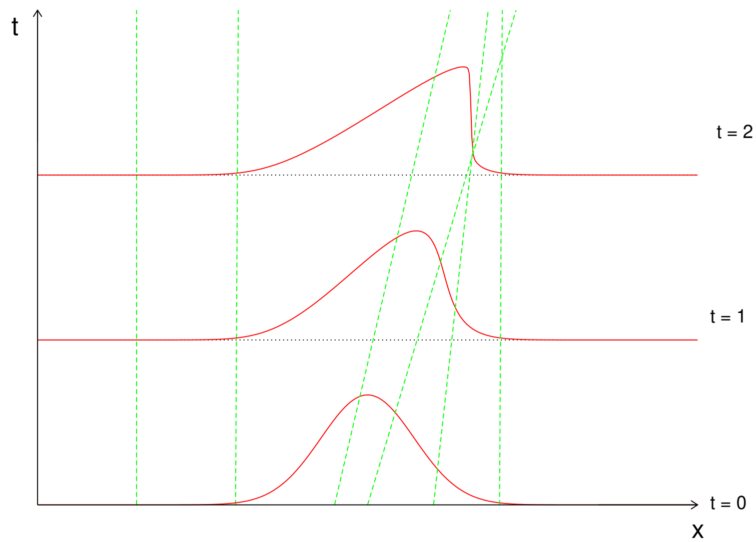


Figure 6: The same Gaussian initial pulse as in Fig. 5 is evolved in time, but now according to Burgers' equation $\partial_t f + f\partial_x f = 0$, i.e. the characteristic speed is now equal to the function value f. Along each characteristic, f remain constant, but now the characteristics will cross in finite time resulting in the formation of a discontinuity or *shock*. As in Fig. 5, the (red) Gaussian curves are not to be regarded as curves in the (t, x) plane, but rather should pop out of the paper.

so the function remains constant along each characteristic curve. The key difference to the advection equation (C.45) is that the slopes of the characteristics now vary with the initial data $f(0, x) = f_0(x)$. This is illustrated by the green dashed curves in Fig. 6 which shows the time evolution of a Gaussian pulse. The characteristics cross in finite time, resulting in a multi valued function, i.e. a discontinuity or *shock*. Rather than being advected across the domain, the Gaussian profile tilts over until its slope becomes vertical. In order to compute the solution beyond this point, one needs to resort to shock capturing schemes that take into account the conservation law underlying the PDE. This topic is outside the scope of our lecture, though, and readers are referred to LeVeque's book [21] for a more detailed introduction to these methods.

C.2.3 *Constant-coefficient first-order systems

Before we engage into the more general class of quasi-linear PDE systems, we consider a simpler type of equations that can be reduced to a set of advection equations. Let $\boldsymbol{f} : \mathbb{R}^2 \to \mathbb{R}^M$ and $\mathbf{A}$ be a constant $M \times M$ matrix. Denoting our coordinates by (t, x), the PDE

$$\partial_t \boldsymbol{f} + \mathbf{A}\partial_x \boldsymbol{f} = 0\,, \qquad \boldsymbol{f}(0, x) = \boldsymbol{f}_0(x)\,, \tag{C.55}$$

then provides us with a *first-order homogeneous PDE system with constant coefficients* with initial data $f_0(x)$.

Def. : The PDE system (C.55) is *hyperbolic* if $\mathbf{A}$ is diagonalizable with real Eigenvalues. If all Eigenvalues are distinct, the system is called *strictly hyperbolic*.

We now use the same notation as in Sec. C.1.2, so let us assume we have a hyperbolic system and denote by $\boldsymbol{V}_{(k)}$ and $\lambda_{(k)}$, respectively, the Eigenvectors and Eigenvalues of $\mathbf{A}$. We assemble the Eigenvectors as column vectors of the new matrix

$$\mathbf{Q} = (Q_{ij}) := \begin{pmatrix} V_{1(1)} & V_{1(2)} & \cdots & V_{1(M)} \\ V_{2(1)} & V_{2(2)} & \cdots & V_{2(M)} \\ \vdots & \vdots & \ddots & \vdots \\ V_{M(1)} & V_{M(2)} & \cdots & V_{M(M)} \end{pmatrix}, \tag{C.56}$$

and define the diagonal matrix

$$\boldsymbol{\Lambda} := \lambda_{(i)}\delta_{ij} = \begin{pmatrix} \lambda_{(1)} & 0 & \cdots & 0 \\ 0 & \lambda_{(2)} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_{(M)} \end{pmatrix}. \tag{C.57}$$

We can always orthonormalize the Eigenvectors and thus make $\mathbf{Q}$ orthogonal, so that $\mathbf{Q}^{-1} = \mathbf{Q}^{\intercal}$ (otherwise replace $\mathbf{Q}^{\intercal}$ with $\mathbf{Q}^{-1}$ in the following), so that the Eigenvector condition gives us

$$\begin{aligned} \mathbf{A}\boldsymbol{V}_{(k)} = \lambda_{(k)}\boldsymbol{V}_{(k)} \qquad &\Rightarrow \qquad \mathbf{A}\mathbf{Q} = \mathbf{Q}\boldsymbol{\Lambda} \\ \Rightarrow \quad \mathbf{A} = \mathbf{Q}\boldsymbol{\Lambda}\mathbf{Q}^{\intercal} \qquad &\Leftrightarrow \qquad \mathbf{Q}^{\intercal}\mathbf{A}\mathbf{Q} = \boldsymbol{\Lambda}\,. \end{aligned} \tag{C.58}$$

Next we introduce *characateristic variables* $\boldsymbol{g} := \mathbf{Q}^{\intercal}\boldsymbol{f}$ and our PDE (C.55) becomes

$$\begin{aligned} &\mathbf{Q}^{\intercal}\partial_t\boldsymbol{f} + \mathbf{Q}^{\intercal}\mathbf{A}\partial_x\boldsymbol{f} = 0 \\ \Rightarrow \quad &\mathbf{Q}^{\intercal}\partial_t\boldsymbol{f} + \boldsymbol{\Lambda}\mathbf{Q}^{\intercal}\partial_x\boldsymbol{f} = 0 \qquad \Big|\ \mathbf{Q} = \text{const} \\ \Rightarrow \quad &\partial_t\boldsymbol{g} + \boldsymbol{\Lambda}\partial_x\boldsymbol{g} = 0\,, \end{aligned} \tag{C.59}$$

or, in components,

$$\partial_t g_i + \lambda_{(i)}\partial_x g_i = 0 \qquad \text{(no summation over } i\text{)} \tag{C.60}$$

This is a system of M decoupled advection equations of the form $\partial_t g + \lambda\partial_x g = 0$ with solutions $g(t,x) = g(0, x - \lambda t)$. The solution to Eq. (C.60) is therefore given by

$$\boxed{g_i(t,x) = g_i(0, x - \lambda_{(i)}t)\,.} \tag{C.61}$$

Next, we recall that

$$\boldsymbol{f} = \mathbf{Q}\boldsymbol{g} \qquad \Leftrightarrow \qquad f_m = Q_{mi}g_i = V_{m(i)}g_i \qquad \text{(Here we sum over } i\text{)}\,. \tag{C.62}$$

So g_i is the ith component of the Eigenvector expansion of $\boldsymbol{f}$. This enables us to write the solution to the PDE (C.55) as

$$f_i(t,x) = Q_{im} g_m(t,x) = Q_{im} g_m(0, x - \lambda_{(m)} t) = g_m(0, x - \lambda_{(m)} t) V_{i(m)} \,. \tag{C.63}$$

In words, find the Eigenvector expansion of the initial data $f_0(x)$. The mth component in this expansion is $g_m(0,x)$, the Eigenvector is $\boldsymbol{V}_{(m)}$ and the Eigenvalue is $\lambda_{(m)}$. The solution to the PDE is then (C.63). The characteristic curves are given by $x - \lambda_{(m)} t = \text{const}$ and there are M such sets of curves.

C.2.4 *Quasi-linear first-order PDE systems

C.2.4.1 *The characteristic equation

We now switch to the physically more important (and interesting) case of quasi-linear first-order PDE systems. We also generalize the domain to more than one spatial dimension. Let us consider for this purpose functions $\boldsymbol{f} : \mathbb{R}^N \to \mathbb{R}^M$. We use the notation

$$\boldsymbol{f} = \begin{pmatrix} f_1 \\ \vdots \\ f_M \end{pmatrix} \,, \qquad \partial_\mu \boldsymbol{f} := \frac{\partial}{\partial x_\mu} \boldsymbol{f} = \begin{pmatrix} \partial_\mu f_1 \\ \vdots \\ \partial_\mu f_M \end{pmatrix} \,, \quad \mu = 1,\, \ldots,\, N \,. \tag{C.64}$$

Def. : The *general quasi-linear first-order PDE* for a function $\boldsymbol{f} : \Omega \subset \mathbb{R}^N \to \mathbb{R}^M$ is

$$\mathbf{A}^\mu(\boldsymbol{x}, \boldsymbol{f}) \partial_\mu \boldsymbol{f} + \boldsymbol{b}(\boldsymbol{x}, \boldsymbol{f}) = 0 \,, \tag{C.65}$$

where $\boldsymbol{b}$ is a vector valued function and each $\mathbf{A}^\mu$, $\mu = 1,\, \ldots,\, N$ is an $M \times M$ matrix. In component notation, we write

$$A^\mu_{mn}(x_\nu, f_i) \partial_\mu f_n + b_m(x_\nu, f_i) = 0 \,, \tag{C.66}$$

where we sum over μ, m and n.

As in our discussion of second-order PDEs in Sec. C.1.1, we next consider a hypersurface S defined as the level set of a function $t(x_\mu) = 0$ with $\nabla t \neq 0$. Let us assume that initial data $\boldsymbol{f}(\boldsymbol{x})$ are specified on S. As before, we ask the question whether or not we can calculate all derivatives of $\boldsymbol{f}$ on S.

As a first step, we introduce adapted coordinates ξ_α as in Eq. (C.4),

$$\begin{aligned} \xi_\alpha &= \xi_\alpha(x^\mu) \qquad \text{for } \alpha = 1,\, \ldots,\, N-1 \,, \\ \xi_N &= t(x^\mu) \,, \end{aligned}$$

so that by chain rule

$$\partial_\mu \boldsymbol{f} = \frac{\partial \boldsymbol{f}}{\partial x_\mu} = \frac{\partial \xi_\alpha}{\partial x_\mu} \frac{\partial \boldsymbol{f}}{\partial \xi_\alpha} = \frac{\partial \xi_\alpha}{\partial x_\mu} \partial_\alpha \boldsymbol{f} \quad \text{with} \quad \mu = 1,\, \ldots,\, N \,. \tag{C.67}$$

In terms of these coordinates, our PDE system (C.65) becomes

$$\mathbf{A}^\mu \partial_\mu \boldsymbol{f} = \mathbf{A}^\mu \frac{\partial \xi_\alpha}{\partial x_\mu} \frac{\partial \boldsymbol{f}}{\partial \xi_\alpha} = -\boldsymbol{b}\,. \tag{C.68}$$

For $\alpha = 1, \ldots, N-1$, the derivatives $\frac{\partial \boldsymbol{f}}{\partial \xi_\alpha}$ can be evaluated from the differential quotients

$$\frac{\partial \boldsymbol{f}}{\partial \xi_\alpha} = \lim_{h\to 0} \frac{\boldsymbol{f}(\xi_1, \ldots, \xi_\alpha + h, \ldots, \xi_{N-1}, 0) - \boldsymbol{f}(\xi_1, \ldots, \xi_{N-1}, 0)}{h}\,, \tag{C.69}$$

as in Eq. (C.8) in our discussion of second-order PDEs. The missing derivative $\frac{\partial \boldsymbol{f}}{\partial \xi_N} = \frac{\partial \boldsymbol{f}}{\partial t}$ is obtained by using the PDE (C.65) which we can write as

$$\mathbf{A}^\mu \frac{\partial t}{\partial x_\mu} \frac{\partial \boldsymbol{f}}{\partial t} = \text{terms known on } S\,. \tag{C.70}$$

Solving for $\frac{\partial \boldsymbol{f}}{\partial t}$ requires inversion of the matrix which, in turn, requires

$$\det\left(\mathbf{A}^\mu \frac{\partial t}{\partial x_\mu}\right) \neq 0\,. \tag{C.71}$$

Note that this condition depends on the coefficient matrices $\mathbf{A}^\mu$ *and* the surface S, i.e. the function $t(x_\mu)$.

Def. : The *characteristic equation* associated with the PDE (C.65) and the level surface S given by $t(x_\mu) = 0$ is

$$\det(\mathbf{A}^\mu \partial_\mu t) = 0\,. \tag{C.72}$$

A level surface S defined through $t(x_\mu) = 0$ by a solution to the characteristic equation is called a *characteristic surface*.

In words, initial data $\boldsymbol{f}(\boldsymbol{x})$ specified on a characteristic surface does *not* allow us to calculate all derivatives and therefore does not determine the solution at any point away from S, no matter how close. Before we proceed with the classification of PDE systems, it will be helpful to acquire at least a modicum of experience about what is going on here.

Examples

(1) The wave equation in $2+1$ dimensions and Cartesian coordinates is

$$-\partial_t^2 g + \partial_x^2 g + \partial_y^2 g = 0\,. \tag{C.73}$$

We convert this equation into a first-order system by defining

$$\psi := \partial_t g\,, \qquad \lambda := \partial_x g\,, \qquad \mu := \partial_y g\,,$$

$$\Rightarrow \quad \partial_t \psi - \partial_x \lambda - \partial_y \mu \quad = \quad 0\,,$$

$$\begin{aligned} \wedge \quad & -\partial_x\psi + \partial_t\lambda & = \ & 0\,, \\ \wedge \quad & -\partial_y\psi \qquad\quad + \partial_t\mu & = \ & 0\,. \end{aligned} \tag{C.74}$$

We note that one subtlety arises in this conversion into a first-order system: We have treated the t coordinate in a preferential way here by using the second-order wave equation in deriving the first-order equation for $\partial_t\psi$, whereas the equations for $\partial_t\lambda$ and $\partial_t\mu$ merely mirror the commutation of partial derivatives. There is nothing wrong with our choice, but we mention it in passing since this freedom may complicate some aspects of analyzing the PDE system.

In the notation of (C.65), the system (C.74) becomes

$$\boldsymbol{f} = \begin{pmatrix} \psi \\ \lambda \\ \mu \end{pmatrix}, \quad \mathbf{A}^t = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \mathbf{A}^x = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathbf{A}^y = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}.$$

Since we have already used the letter 't' as a coordinate here, we label the level surfaces by the function $\theta(t,x,y)$ and obtain the characteristic equation

$$\det(\mathbf{A}^\mu\partial_\mu\theta) = \begin{vmatrix} \partial_t\theta & -\partial_x\theta & \partial_y\theta \\ -\partial_x\theta & \partial_t\theta & 0 \\ -\partial_y\theta & 0 & \partial_t\theta \end{vmatrix} = \ldots = \partial_t\theta\left[(\partial_t\theta)^2 - (\partial_x\theta)^2 - (\partial_y\theta)^2\right]. \tag{C.75}$$

(2) For the Laplace equation in 3 dimensions,

$$\partial_x^2 g + \partial_y^2 g + \partial_z^2 g = 0\,, \tag{C.76}$$

we proceed in complete analogy as for the wave equation. Besides the relabeling of the coordinates from (t,x,y) to (x,y,z), the only change is that all '$-$' signs turn into '$+$' signs and we obtain the characteristic equation

$$\det(\mathbf{A}^\mu\partial_\mu\theta) = \partial_x\theta\left[(\partial_x\theta)^2 + (\partial_y\theta)^2 + (\partial_z\theta)^2\right]. \tag{C.77}$$

(3) The heat equation in 2+1 dimensions,

$$-\partial_t g + \partial_x^2 g + \partial_y^2 g = 0\,, \tag{C.78}$$

is a little different since we have no second derivative in t. Still, we can proceed largely as in the case of the wave equation and define

$$\psi := \partial_t g\,, \qquad \lambda := \partial_x g\,, \qquad \mu := \partial_y g\,,$$

$$\begin{aligned} \Rightarrow \quad & -\partial_x\lambda - \partial_y\mu & = \ & -\psi\,, \\ \wedge \quad & \partial_t\lambda - \partial_x\psi & = \ & 0\,, \end{aligned}$$

$$\wedge \quad \partial_t \mu \qquad\qquad - \partial_y \psi \;\; = \;\; 0\,. \tag{C.79}$$

The appearance of $-\psi$ on the right-hand side is inconsequential for the existence or absence of characteristic surfaces and therefore plays no further role in our analysis. In the matrix notation of (C.65), we have

$$\boldsymbol{f} = \begin{pmatrix} \psi \\ \lambda \\ \mu \end{pmatrix}\,, \quad \mathbf{A}^t = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\,, \quad \mathbf{A}^x = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\,, \quad \mathbf{A}^y = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}\,,$$

and the characteristic equation is given by

$$\det(\mathbf{A}^\mu \partial_\mu \theta) = \begin{vmatrix} 0 & -\partial_x\theta & \partial_y\theta \\ -\partial_x\theta & \partial_t\theta & 0 \\ -\partial_y\theta & 0 & \partial_t\theta \end{vmatrix} = \ldots = -\partial_t\theta \left[(\partial_x\theta)^2 + (\partial_y\theta)^2\right]\,. \tag{C.80}$$

C.2.4.2 *Classification of first-order PDE systems

We now return to the characteristic equation (C.72) and interpret its gradient solutions $\partial_\mu t$. This gradient is associated with the level surfaces $t(x_\mu) = \text{const}$ by defining at every point x_μ the direction normal to the surface. We can thus interpret the characteristic equation as the search for the normal directions of surfaces on which initial data will not be sufficient to compute all derivatives of the function $\boldsymbol{f}$. We therefore introduce a vector (or one-form) field ζ_μ and define

$$C(\boldsymbol{x}, \boldsymbol{f}, \boldsymbol{\zeta}) \coloneqq \det\left[\mathbf{A}^\mu(\boldsymbol{x}, \boldsymbol{f})\zeta_\mu\right]\,. \tag{C.81}$$

For the classification of PDEs, it turns out convenient to express the directions $\boldsymbol{\zeta}$ in a more general form as a linear function of N parameters, i.e. introduce a linear mapping

$$\boldsymbol{\zeta} = \mathbf{M}\boldsymbol{\eta}\,, \quad \text{where} \quad \boldsymbol{\eta} = (\eta_1,\, \ldots,\, \eta_{N-1},\, \kappa)\,, \tag{C.82}$$

with a non-degenerate matrix $\mathbf{M}$, and write

$$C(\boldsymbol{x}, \boldsymbol{f}, \boldsymbol{\eta}) = C(\boldsymbol{x}, \boldsymbol{f}, \eta_1, \ldots, \eta_{N-1}, \kappa) \coloneqq C\Big(\boldsymbol{x}, \boldsymbol{f}, \boldsymbol{\zeta}(\eta_1, \ldots, \eta_{N-1}, \kappa)\Big)\,. \tag{C.83}$$

The purpose of allowing for this generic reparametrization of the directional vector $\boldsymbol{\zeta}$ is that we wish to single out a specific parameter κ that does not necessarily coincide with an actual component of $\boldsymbol{\zeta}$ in our original coordinate system.

Def. : The general quasi-linear first-order PDE system (C.65) is

- *hyperbolic* at $\boldsymbol{x}$ if there exists a regular linear mapping $\boldsymbol{\zeta} = \mathbf{M}\boldsymbol{\eta}$, such that there exist M *real* roots $\kappa_i = \kappa_i(\boldsymbol{x}, \boldsymbol{f}(\boldsymbol{x}), \eta_1, \ldots, \eta_{N-1})$, $i = 1, \ldots, M$ of $C(\boldsymbol{x}, \boldsymbol{f}, \boldsymbol{\eta}) = 0$ for all $(\eta_1, \ldots, \eta_{n-1})$. Note that the number of roots required equals the number of independent variables in $\boldsymbol{f}$, not the dimensionality N of the domain.

- *parabolic* at $\boldsymbol{x}$ if there exists a linear mapping $\boldsymbol{\zeta} = \mathbf{M}\boldsymbol{\eta}$ such that C is independent of κ, i.e. depends on fewer than N parameters.

- *elliptic* if $C(\boldsymbol{x}, \boldsymbol{f}, \boldsymbol{\zeta}) = 0$ only if $\boldsymbol{\zeta} = 0$.

If you find this definition a bit cryptic, that makes two of us. Let us try our best to interpret the three cases. The elliptic case is intuitively the most obvious: $\det[\mathbf{A}^\mu(\boldsymbol{x}, \boldsymbol{f})\zeta_\mu]$ is non-zero for any non-vanishing gradient $\partial_\mu t$, so that there exist no characteristic surfaces. That means for any initial surface S, we can determine all derivatives and, thus, the solution in some neighbourhood of S. Loosely speaking, the hyperbolic case implies that we can find for each function f_i a characteristic surface. The parabolic case, to me, is rather shrouded in mist. I should note, at this point, that I have as yet not come across a situation where I had to apply this definition in practice. Let us instead acquire some familiarity by discussing examples and comparing this definition with the simpler cases we have discussed above.

Examples

(1) For the advection equation equation

$$\partial_t f + \partial_x f = 0\,, \tag{C.84}$$

the matrices $\mathbf{A}^\mu$ are in fact trivial scalars,

$$\mathbf{A}^1 = 1\,, \qquad \mathbf{A}^2 = 1\,; \tag{C.85}$$

the superscripts are, of course, not exponents here, but correspond to $\mu = 1$ and $\mu = 2$ in $\mathbf{A}^\mu$. For $\boldsymbol{\zeta} = (\zeta_1, \zeta_2)$, the characteristic equation gives us

$$C = \det\left(\mathbf{A}^1\zeta_1 + \mathbf{A}^2\zeta_2\right) = \zeta_1 + \zeta_2 = 0\,. \tag{C.86}$$

Just setting $\zeta_1 = \eta_1$, $\zeta_2 = \kappa$, we get $\eta_1 + \kappa = 0$ which for any η_1 has one real root $\kappa = -\eta_1$; the advection equation is hyperbolic.

(2) The wave equation with propagation speed c in one spatial dimension is given by

$$\partial_t^2 f - c^2\partial_x^2 f = 0\,, \tag{C.87}$$

and can be converted into a first-order system according to Eq. (C.74) by introducing $\psi \coloneqq \partial_t f$, $\lambda \coloneqq \partial_x f$ which gives us

$$\partial_t \begin{pmatrix}\psi \\ \lambda\end{pmatrix} + \begin{pmatrix}-c^2\partial_x\lambda \\ -\partial_x\psi\end{pmatrix} = \begin{pmatrix}1 & 0 \\ 0 & 1\end{pmatrix}\partial_t\begin{pmatrix}\psi \\ \lambda\end{pmatrix} + \begin{pmatrix}0 & -c^2 \\ -1 & 0\end{pmatrix}\partial_x\begin{pmatrix}\psi \\ \lambda\end{pmatrix} = 0$$

$$\Rightarrow \quad \mathbf{A}^1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad \mathbf{A}^2 = \begin{pmatrix} 0 & -c^2 \\ -1 & 0 \end{pmatrix}$$

$$\Rightarrow \quad \det(\mathbf{A}^\mu \zeta_\mu) = \begin{vmatrix} \zeta_1 & -c^2\zeta_2 \\ -\zeta_2 & \zeta_1 \end{vmatrix} = \zeta_1^2 - c^2\zeta_2^2 \,. \tag{C.88}$$

Again, we set $\zeta_1 = \eta_1$, $\zeta_2 = \kappa$, so that the characteristic equation becomes

$$C = \eta_1^2 - c^2\kappa^2 = 0 \qquad \Rightarrow \qquad \kappa = \pm\sqrt{\frac{\eta_1^2}{c^2}}\,, \tag{C.89}$$

i.e. we have two real roots and the wave equation is hyperbolic.

(3) For the 2D Laplace equation $\partial_x^2 f + \partial_y^2 f$, we similarly introduce $F := \partial_x f$, $G := \partial_y f$, so that $\partial_x F = -\partial_y G$ and $\partial_x G = \partial_y F$ or

$$\partial_x \begin{pmatrix} F \\ G \end{pmatrix} + \partial_y \begin{pmatrix} G \\ -F \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \partial_x \begin{pmatrix} F \\ G \end{pmatrix} + \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \partial_x \begin{pmatrix} F \\ G \end{pmatrix}$$

$$\Rightarrow \quad \det\left(\mathbf{A}^1\zeta_1 + \mathbf{A}^2\zeta_2\right) = \begin{vmatrix} \zeta_1 & \zeta_2 \\ -\zeta_2 & \zeta_1 \end{vmatrix} = \zeta_1^2 + \zeta_2^2 = 0\,, \tag{C.90}$$

which only has the trivial solution $\zeta_1 = \zeta_2 = 0$. Newsflash: the Laplace equation is elliptic.

(4) The 1+1 dimensional heat equation $-\partial_t f + \partial_x^2 f = 0$ is converted into a first-order system in analogy to Eq. (C.79) for the 2+1 dimensional case by defining $\psi := \partial_t f$, $\lambda := \partial_x f$. This gives us

$$\begin{pmatrix} 0 \\ \partial_t\lambda \end{pmatrix} + \begin{pmatrix} -\partial_x\lambda \\ -\partial_x\psi \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \partial_t \begin{pmatrix} \psi \\ \lambda \end{pmatrix} + \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \partial_x \begin{pmatrix} \psi \\ \lambda \end{pmatrix} = \begin{pmatrix} -\psi \\ 0 \end{pmatrix}$$

$$\Rightarrow \quad \mathbf{A}^t = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \qquad \mathbf{A}^x = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$$

$$\Rightarrow \quad \det(\mathbf{A}^\mu\zeta_\mu) = \begin{vmatrix} 0 & -\zeta_2 \\ -\zeta_2 & \zeta_1 \end{vmatrix} = -\zeta_x^2 \,. \tag{C.91}$$

Setting $\zeta_t = \kappa$, $\zeta_2 = \eta_1$, we see that $C(\boldsymbol{x}, \boldsymbol{f}, \boldsymbol{\eta})$ is independent of κ.

So what does this mean? Clearly any characteristic direction requires $\zeta_2 = \zeta_x = 0$, but we can choose $\zeta_1 = \zeta_t$ arbitrarily, so that all solutions are of the form $\boldsymbol{\zeta} = (\kappa, 0)$ and the characteristic surfaces are just $t = \text{const}$.

(5) For the constant-coefficient first-order systems we have discussed in Sec. C.2.3, we defined hyperbolicity in a rather different way using the Eigenvalues of the coefficient matrix $\mathbf{A}$ in Eq. (C.55). How does that square with the definition used here?

This is most easily addressed by considering the PDE in its (fully equivalent) normal form (C.59) which immediately gives us

$$\mathbf{A}^t = \boldsymbol{I}\,, \qquad \mathbf{A}^x = \boldsymbol{\Lambda}\,. \tag{C.92}$$

This gives us

$$\det(\mathbf{A}^\mu \zeta_\mu) = \begin{vmatrix} \zeta_t + \lambda_{(1)}\zeta_x & 0 & \cdots & 0 \\ 0 & \zeta_t + \lambda_{(2)}\zeta_x & \cdots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \cdots & \zeta_t + \lambda_{(M)}\zeta_x \end{vmatrix} = \prod_{i=1}^{M} (\zeta_t + \lambda_{(i)}\zeta_x) = 0\,. \tag{C.93}$$

The Eigenvalues are real since we assume our constant coefficient system to be hyperbolic. Setting $\zeta_t = \kappa$ and $\zeta_x = \eta_1$, we therefore obtain M real roots κ of the characteristic equation and our system is also hyperbolic according to the generalized definition.

D The structure of the Einstein equations

In this section, we will analyze in some detail the structure of the field equations of general relativity or, to be more precise, of the gravitational sector of the equations

$$G_{\alpha\beta} = 8\pi T_{\alpha\beta}\,,$$

Expressed in a coordinate chart x^α, these equations constitute a set of 10 second-order, non-linear PDEs. We can view these differential equations from three different angles.

(1) Given a matter distribution $T_{\alpha\beta}$, we search for the metric components $g_{\alpha\beta}$ satisfying the Einstein equations. For example, this is the view we take in solving the vacuum field equations (A.5).

(2) We can freely choose the metric $g_{\alpha\beta}$, compute by recipe the resulting Einstein tensor $G_{\alpha\beta}$ which gives us the matter distribution corresponding to the metric. This approach is rarely useful in practice, since the resulting $T_{\alpha\beta}$ will almost invariably be unphysical.

(3) The 10 Einstein equations (A.4) relate 20 quantities, 10 metric components $g_{\alpha\beta}$ and 10 components of the energy momentum tensor $T_{\alpha\beta}$. Here we regard the Einstein equations as 10 constraints on simultaneous choices of $g_{\alpha\beta}$ and $T_{\alpha\beta}$.

In the following discussion, we shall focus on the geometric sector of general relativity and therefore largely work with the vacuum equations. By virtue of the Bianchi identities, we immediately see that the energy-momentum tensor is conserved,

$$\nabla_\mu T^\mu{}_\alpha = 0\,, \tag{D.1}$$

and the modelling of the matter sources involves a lot of new challenges such as shock capturing, equations of state etc. These, however, intricately depend on the specific matter systems under consideration and we could probably organize a separate lecture course for each type of matter. Furthermore, these challenges are quite different in nature from those associated with the evolution of the spacetime geometry.

D.1 The Einstein equations in vacuum

We have already seen above that we can write the vacuum field equations of general relativity as $G_{\alpha\beta} = 0$ or, fully equivalently, as $R_{\alpha\beta} = 0$. Our first observation is that the field equations are not independent; the $G_{\alpha\beta}$ must satisfy the contracted Bianchi identities (A.3) and we seem to have too few equations to determine all 10 components of the spacetime metric $g_{\alpha\beta}$. This should not surprise us given the coordinate freedom of general relativity; the metric components $g_{\alpha\beta}$ cannot be fully determined by physical considerations since we can change coordinates according to $\tilde{x}^\alpha = \tilde{x}^\alpha(x^\mu)$ to obtain new metric components

$$\tilde{g}_{\tilde{\alpha}\tilde{\beta}} = \frac{\partial x^\mu}{\partial \tilde{x}^\alpha}\frac{\partial x^\nu}{\partial \tilde{x}^\beta} g_{\mu\nu}\,, \tag{D.2}$$

without altering the spacetime. For example, we could choose the four coordinates such that $g_{00} = 1$ and $g_{0i} = 0$ everywhere. The six independent Einstein equations would then determine the six remaining metric components g_{ij}. We will see this more explicitly further below when we discuss the 3+1 split of the Einstein equations.

In our discussion, we will generally assume that solutions $g_{\alpha\beta}$ to the Einstein equations are infinitely differentiable, i.e. C^∞ functions, but we note that this assumption can be weakened to merely require the metric functions to be C^2, i.e. twice differentiable. This occurs in practice when we have discontinuities in the matter sources $T_{\alpha\beta}$ as for example in shock forming fluids.

D.2 The Cauchy problem

The Cauchy problem is formally defined as the process of constructing a solution to a PDE given data on some boundary or initial hypersurface. In the context of the Einstein equations, this implies the evolution in time of a specified initial snapshot, as for example two black holes at rest separated by some initial distance. We emphasize that the formulation of the Einstein equations as a Cauchy problem is far less obvious than for many systems in Newtonian dynamics since we do not even know a-priori whether we have a time coordinate and whether some candidate time is timelike throughout the spacetime. All we know is that the signature of the Lorentzian metric is +2 and thus in principle admits one timelike direction. We start this discussion with a few definitions.

Def. : Let $\mathcal{M}$ be a Lorentzian manifold $\mathcal{M}$ with metric $g_{\alpha\beta}$ of signature $+2$.

A *Cauchy surface* is a spacelike hypersurface Σ in $\mathcal{M}$ such that each timelike or null curve without endpoints intersects Σ exactly once.

The spacetime $(\mathcal{M}, \boldsymbol{g})$ is *globally hyperbolic* if it admits a Cauchy surface.

Without proof, we note the following important result.

Proposition: Let Σ be a Cauchy surface of a globally hyperbolic spacetime $(\mathcal{M}, \boldsymbol{g})$. Then there exists a smooth function

$$t : \mathcal{M} \to \mathbb{R} \qquad \text{with} \qquad \mathbf{d}t \neq 0\,, \tag{D.3}$$

such that Σ is a level surface

$$\Sigma_{t_0} := \{p \in \mathcal{M} \quad : \quad t(p) = t_0\}\,, \tag{D.4}$$

and two level surfaces Σ_{t_1} and Σ_{t_2} are either disjoint or equal,

$$\Sigma_{t_1} \cap \Sigma_{t_2} = \emptyset \qquad \Leftrightarrow \qquad t_1 \neq t_2\,. \tag{D.5}$$

Def. : If $(\mathcal{M}, \boldsymbol{g})$ is a globally hyperbolic spacetime and $\mathcal{M} = \bigcup_{t\in\mathbb{R}} \Sigma_t$, then the union of the Σ_t is called a *foliation* of the spacetime.

Figure 7: Illustration of a foliation Σ_t of a spacetime $(\mathcal{M}, \boldsymbol{g})$. Time points upwards and one of the three spatial dimensions is suppressed.

A graphical illustration of a foliation is shown in Fig. 7. Let us now assume that we have a globally hyperbolic spacetime with hypersurface Σ_0 given by $t(x^\alpha) = 0$ and that $||\mathbf{d}t||^2 < 0$, i.e. Σ is spacelike. We can then promote t to a coordinate, say, $x^0 := t$ and specify the remaining coordinates x^i such that they label on each hypersurface Σ_t the points inside this three-dimensional submanifold. We now ask the same question as in Sec. C.1.1 when we attempted to classify PDEs: Given the metric $g_{\alpha\beta}$ and its first derivatives $\partial_\gamma g_{\alpha\beta}$ on a hypersurface Σ_0, can we determine through the Einstein field equations all derivatives of $g_{\alpha\beta}$ on Σ_0? If yes, the time evolution of these initial data is determined at least in some neighbourhood of Σ_0.

As in Sec. C.1.1, the potentially problematic derivative is $\partial_0^2 g_{\alpha\beta}$. In simple terms, we wish to solve the Einstein equations for $\partial_0^2 g_{\alpha\beta}$. We consider for this purpose the vacuum equations in the form $R_{\alpha\beta} = 0$.

(1) We first compute the component R_{00}. From the definitions (A.1), we obtain

$$R_{00} = R^\mu{}_{0\mu 0} = R^0{}_{000} + R^m{}_{0m0}$$

$$R^0{}_{000} = 0\,,$$

$$R^m{}_{0m0} = \partial_m \Gamma^m_{00} - \partial_0 \Gamma^m_{0m} + \text{“}\Gamma \times \Gamma\text{”}, \tag{D.6}$$

where by $\Gamma \times \Gamma$ we denote the third and fourth terms in the definition (A.1) of the Riemann tensor. The Christoffel symbols $\Gamma^\rho_{\mu\nu}$ only involve first derivatives of the metric and are therefore known on Σ_0; their explicit form is inconsequential for the question at hand. Next, we note that the term $\partial_m \Gamma^m_{00}$ involves at most one time derivative of the metric and is therefore also known on Σ_0. That leaves us with

$$\partial_0 \Gamma^m_{0m} \quad = \quad \partial_0 \left[\frac{1}{2} g^{m\rho} \left(\partial_0 g_{m\rho} + \partial_m g_{\rho 0} - \partial_\rho g_{0m}\right)\right]$$

$$\begin{aligned}\Rightarrow R_{00} &= -\frac{1}{2}g^{m\rho}\partial_0^2 g_{m\rho} + \frac{1}{2}g^{m0}\partial_0^2 g_{0m} + M_{00} \\ &= -\frac{1}{2}g^{mn}\partial_0^2 g_{mn} + M_{00}\,,\end{aligned} \tag{D.7}$$

where we have introduced M_{00} as a garbage collector for all terms involving at most first derivatives in time, which are known on Σ_0.

(2) We likewise obtain for the mixed space-time components,

$$R_{0i} = R^{\mu}{}_{0\mu i} = R^{0}{}_{00i} + R^{m}{}_{0mi}$$

$$R^{0}{}_{00i} = \partial_0\Gamma^0_{0i} + \text{l.o.t.}\,, \qquad R^{m}{}_{0mi} = \text{l.o.t.}\,,$$

where l.o.t. stands for "lower-order terms" involving at most first time derivatives. The only relevant term is

$$\begin{aligned}\partial_0\Gamma^0_{0i} &= \partial_0\left[\frac{1}{2}g^{0\rho}(\partial_0 g_{i\rho} + \partial_i g_{\rho 0} - \partial_\rho g_{0i})\right] \\ \Rightarrow R_{0i} &= \frac{1}{2}g^{00}\partial_0^2 g_{i0} + \frac{1}{2}g^{0m}\partial_0^2 g_{im} - \frac{1}{2}g^{00}\partial_0^2 g_{0i} + \text{l.o.t.} \\ &= \frac{1}{2}g^{0m}\partial_0^2 g_{im} + M_{0i}\,,\end{aligned} \tag{D.8}$$

where M_{0i} is the depository for all lower-order terms analogous to the above M_{00}.

(3) Finally, we have the spatial components

$$\begin{aligned}R_{ij} &= R^{\mu}{}_{i\mu j} = R^{0}{}_{i0j} + R^{m}{}_{imj} = \partial_0\Gamma^0_{ij} + \text{l.o.t.} \\ &= \partial_0\left[\frac{1}{2}g^{0\rho}(\partial_i g_{j\rho} + \partial_j g_{\rho i} - \partial_\rho g_{ij})\right] \\ &= -\frac{1}{2}g^{00}\partial_0^2 g_{ij} + M_{ij}\,,\end{aligned} \tag{D.9}$$

with M_{ij} denoting at most first-order-in-time terms as before.

We can summarize our findings as follows.

(i) We have no terms $\partial_0^2 g_{0\alpha}$, so the time evolution of the components $g_{0\alpha}$ is *not* determined by the Einstein equations.

(ii) We have 10 equations for the 6 unknowns $\partial_0^2 g_{ij}$.

We have already seen that the first result follows from the coordinate or *gauge* freedom of general relativity. The second result demonstrates that the metric must obey some constraints. We will derive these constraint equations more concretely in the 3+1 split in Sec. F, but we can already gain some insight by investigating the expressions (D.7)-(D.9) for the Ricci tensor.

Assuming that[3] $g^{00} \neq 0$, Eq. (D.9) can be solved for the missing second time derivatives $\partial_0^2 g_{ij}$; we can thus regard Eq. (D.9) as providing us with the time evolution of the metric components g_{ij}. Next, by taking appropriate linear combinations of all three equations, we find

$$\begin{aligned} g^{00}R_{00} - g^{mn}R_{mn} &= g^{00}M_{00} - g^{mn}M_{mn} = 0\,, \\ g^{00}R_{0i} + g^{0m}R_{im} &= g^{00}M_{0i} + g^{0m}M_{im} = 0\,. \end{aligned} \tag{D.10}$$

Now, if the evolution equations $R_{mn} = 0$ are satisfied, then the vanishing of $R_{00} = R_{0i} = 0$ is equivalent to the vanishing of terms that only involve $M_{\alpha\beta}$, which are completely determined by the initial data. In other words, $R_{00} = R_{0i} = 0$ provide us with constraints that the initial data must satisfy if they correspond to a solution of the Einstein equations. We can alternatively express these constraints in terms of the Einstein tensor. For this purpose, we first use Eqs. (D.7)-(D.9) to write the Ricci scalar as

$$\begin{aligned} R = g^{\mu\nu}R_{\mu\nu} &= g^{00}R_{00} + 2g^{0m}R_{0m} + g^{mn}R_{mn} \\ &= -\frac{1}{2}g^{00}g^{mn}\partial_0^2 g_{mn} + g^{00}M_{00} + g^{0m}g^{0n}\partial_0^2 g_{nm} + 2g^{0n}M_{0n} - \frac{1}{2}g^{mn}g^{00}\partial_0^2 g_{mn} + g^{mn}M_{mn} \\ &= -g^{00}g^{mn}\partial_0^2 g_{mn} + g^{0m}g^{0n}\partial_0^2 g_{mn} + g^{00}M_{00} + 2g^{0m}M_{0m} + g^{mn}M_{mn}\,. \end{aligned} \tag{D.11}$$

For the Einstein tensor we thus obtain

$$\begin{aligned} G_{\alpha\beta} &= R_{\alpha\beta} - \frac{1}{2}g_{\alpha\beta}R \\ \Rightarrow G_0{}^0 &= R_0{}^0 - \frac{1}{2}\delta_0{}^0 R = g^{0\mu}R_{0\mu} - \frac{1}{2}R = g^{00}R_{00} + g^{0m}R_{0m} - \frac{1}{2}R \\ &= -\frac{1}{2}g^{mn}g^{00}\partial_0^2 g_{mn} + g^{00}M_{00} + \frac{1}{2}g^{0m}g^{0n}\partial_0^2 g_{mn} + g^{0m}M_{0m} - \frac{1}{2}R \\ &= g^{00}M_{00} + g^{0m}M_{0m} - \frac{1}{2}g^{00}M_{00} - g^{0m}M_{0m} - \frac{1}{2}g^{mn}M_{mn} \\ \Rightarrow G_0{}^0 &= \frac{1}{2}g^{00}M_{00} - \frac{1}{2}g^{mn}M_{mn}\,. \end{aligned} \tag{D.12}$$

We likewise find

$$\begin{aligned} G_i{}^0 &= g^{00}R_{i0} + g^{0m}R_{im} \\ &= \frac{1}{2}g^{00}g^{0m}\partial_0^2 g_{im} + g^{00}M_{0i} - \frac{1}{2}g^{0m}g^{00}\partial_0^2 g_{im} + g^{0m}M_{im} \end{aligned}$$

[3] The special case where $g^{00} = 0$ leads to the characteristic formulation of the Einstein equations and will be discussed in detail in Sec. E.

$$\Rightarrow G_i{}^0 \;=\; g^{00}M_{0i} + g^{0m}M_{im}\,, \tag{D.13}$$

so that Eq. (D.10) is equivalent to

$$G_0{}^0 = 0 \quad \wedge \quad G_i{}^0 = 0\,, \qquad \text{i.e.} \qquad G_\alpha{}^0 = 0\,. \tag{D.14}$$

We can thus summarize the Einstein equations as the six evolution equations $R_{mn} = 0$ plus four constraints $G_\alpha{}^0 = 0$.

An important relation between the constraint and evolution equations arises from the Bianchi identities (A.3) which can be regarded as *integrability conditions* of the Einstein equations.

Proposition : Let Σ be a Cauchy surface of a globally hyperbolic spacetime $(\mathcal{M}, \boldsymbol{g})$. If the constraints $G_\alpha{}^0 = 0$ are satisfied on Σ and the evolution equations $R_{mn} = 0$ are satisfied on $\mathcal{M}$, then the constraints are satisfied at all times by virtue of the Bianchi identities.

Proof. This proof is not particularly inspiring and we include it here mostly because the theorem plays an important role in *free* numerical evolutions of the Einstein equations, i.e. time evolutions where one does not actively enforce the constraints through elliptic solving. Our strategy will be to first show that all components of the components $G_\alpha{}^\beta$ are linear functions of the components $G_\alpha{}^0$. This enables us to convert the contracted Bianchi identities $\nabla_\mu G_\alpha{}^\mu$ into a set of time evolution equations $\partial_0 G_\alpha{}^0$, which has a unique solution by the theorems of PDEs. $G_\alpha{}^0 = 0$ is a solution and hence the only solution and the constraints hold everywhere.

Here is the long version. We start with the assumption that $R_{ij} = 0$ everywhere. The definition of the Einstein tensor $G_{\alpha\beta} = R_{\alpha\beta} - \frac{1}{2}g_{\alpha\beta}R$ then gives us

$$\begin{aligned} G_0{}^0 &= g^{0\mu}R_{0\mu} - \frac{1}{2}\delta_0{}^0 g^{\mu\nu}R_{\mu\nu} \\ &= g^{00}R_{00} + g^{0m}R_{0m} - \frac{1}{2}\Big(g^{00}R_{00} + g^{0n}R_{0n} + g^{m0}R_{m0} + g^{mn}\underbrace{R_{mn}}_{=0}\Big) \\ &= \frac{1}{2}g^{00}R_{00}\,, \end{aligned} \tag{D.15}$$

$$G_i{}^0 \;=\; g^{0\mu}R_{i\mu} - \frac{1}{2}\delta_i{}^0 R \;=\; g^{0m}\underbrace{R_{im}}_{=0} + g^{00}R_{0i} \;=\; g^{00}R_{0i}\,, \tag{D.16}$$

$$G_0{}^i \;=\; g^{i\mu}R_{0\mu} - 0 \;=\; g^{im}R_{0m} + g^{i0}R_{00}\,, \tag{D.17}$$

$$G_j{}^i \;=\; G^{i\mu}R_{j\mu} - \frac{1}{2}\delta_j{}^i\Big(g^{00}R_{00} + 2g^{0m}R_{0m}\Big) \;=\; g^{i0}R_{j0} - \frac{1}{2}\Big(g^{00}R_{00} + 2g^{0m}R_{0m}\Big) \tag{D.18}$$

Since our initial hypersurface Σ is time like, we have $g^{00} \neq 0$. We can then use the above relations to write

$$G_0{}^i \overset{(D.17)}{=} g^{im} R_{0m} + g^{i0} R_{00} \overset{(D.15),(D.16)}{=} g^{im}(g^{00})^{-1} G_m{}^0 + g^{i0}(g^{00})^{-1}\, 2G_0{}^0 \,, \tag{D.19}$$

$$\begin{aligned} G_j{}^i &\overset{(D.18)}{=} g^{i0} R_{j0} - \frac{1}{2}\delta_j{}^i \Big(g^{00} R_{00} + 2 g^{0m} R_{0m} \Big) \\ &\overset{(D.15),(D.16)}{=} g^{i0}(g^{00})^{-1} G_j{}^0 - \frac{1}{2}\delta_j{}^i \Big[2G_0{}^0 + 2g^{0m}(g^{00})^{-1} G_m{}^0 \Big] \,. \end{aligned} \tag{D.20}$$

So the components $G_\alpha{}^i$ are linear functions of the components $G_\alpha{}^0$ with coefficients that involve only the metric components.

Now we use the contracted Bianchi identities

$$\nabla_\mu G_\alpha{}^\mu = \partial_\mu G_\alpha{}^\mu - \Gamma^\rho_{\alpha\mu} G_\rho{}^\mu + \Gamma^\mu_{\rho\mu} G_\alpha{}^\rho \,. \tag{D.21}$$

The only term containing derivatives of $G_\alpha{}^0$ is the first on the right-hand side,

$$\partial_\mu G_\alpha{}^\mu = \partial_0 G_\alpha{}^0 + \partial_m G_\alpha{}^m \,, \tag{D.22}$$

so that the contracted Bianchi identities become

$$\begin{aligned} 0 = \nabla_\mu G_\alpha{}^0 &= \partial_\mu G_\alpha{}^0 - \Gamma^\rho_{\alpha 0} G_\rho{}^0 - \Gamma^\rho_{\alpha m} G_\rho{}^m + \Gamma^\mu_{0\mu} G_\alpha{}^0 + \Gamma^\mu_{m\mu} G_\alpha{}^m \\ &= \partial_0 G_\alpha{}^0 + \partial_m \underbrace{G_\alpha{}^m}_{\sim G_\alpha{}^0} - \Gamma^\rho_{\alpha 0} G_\rho{}^0 - \Gamma^\rho_{\alpha m} \underbrace{G_\rho{}^m}_{\sim G_\rho{}^0} + \Gamma^\mu_{0\mu} G_\alpha{}^0 + \Gamma^\mu_{m\mu} \underbrace{G_\alpha{}^m}_{\sim G_\alpha{}^0} \\ \Rightarrow \partial_0 G_\alpha{}^0 &= C^{n\mu}{}_\alpha \partial_n G_\mu{}^0 + D^\mu{}_\alpha G_\mu{}^0 \,, \end{aligned} \tag{D.23}$$

where $C^{n\mu}{}_\alpha$ and $D^\mu{}_\alpha$ depend only on the metric and its first derivatives. Equation (D.23) is a PDE determining the time evolution of the functions $G_\alpha{}^0$. By the Cauchy-Kovalevskaya theorem, the differential equation has a unique solution and, since $G_\alpha{}^0 = 0$ on Σ, this solution is given by $G_\alpha{}^0 = 0$ everywhere. □

In numerical simulations, this result does not entirely safe us, however, since any numerical implementation will have some finite error – round-off error at best. The resulting constraint violations can grow over time and even result in numerical instability. We'll discuss ways to mitigate and control this issue in Sec. G.

E The Bondi-Sachs formalism

E.1 Characteristic coordinates

The study of GWs in the framework of fully non-linear GR is most conveniently formulated in terms of characteristic coordinates. This may appear a bit surprising, since we have seen in Sec. C that initial data on characteristic surfaces do not suffice to determine the evolution in its neighbourhood. This does not debar characteristic approaches from use in the evolution of hyperbolic PDEs, however; the missing information in this case is provided in the form of boundary conditions. This can be achieved either through explicit mathematical expressions for the variables or by employing a hybrid approach where part of the domain is evolved as a Cauchy problem using time and spatial coordinates and the remainder with a characteristic formulation. The latter method has been studied in the context of GR and is known as *Cauchy-characteristic matching* or *CCM*. We will briefly return to this concept further below but need not concern ourselves with the details; for our purposes it will be sufficient to assume that the boundary information can be obtained through such means.

The key advantage of a characteristic approach is the simplification it typically bestows upon the structure of PDE systems; cf. the wave equation (C.41). We likewise obtain a remarkably clear structure of the Einstein equations of GR which enables us to interpret the nature of GWs in a fully non-linear framework.

We start this development by constructing a specific set of coordinates adapted to the characteristic structure of the Einstein equations. Recall for this purpose from Eqs. (C.9)-(C.11) that the characteristic surface is a surface where we cannot directly evaluate all higher derivatives by just using initial data and the PDE system. In short, the problem is that we cannot evaluate the second time derivative $\partial_t^2 f$. In the case of the Einstein equations, we identify the very same problem in Eq. (D.9) which we can rewrite as

$$g^{00}\partial_0^2 g_{ij} = 2M_{ij}\,. \tag{E.1}$$

Here, M_{ij} denotes the collection of all terms involving at most first-order derivatives of the metric in time $x^0 = t$. Clearly the condition for solving this equation for $\partial_0^2 g_{ij}$ is $g^{00} \neq 0$. In other words, the characteristic surfaces of the Einstein equations are surfaces where $g^{00} = 0$, i.e. the coordinate x^0 is chosen such that $x^0 = \text{const}$ are null surfaces or, equivalently, x^0 is a null rather than a timelike coordinate. The normal direction to these surfaces is given by the one-form $\mathbf{d}x^0$ with

$$||\mathbf{d}x^0||^2 = \boldsymbol{g}(\mathbf{d}x^0, \mathbf{d}x^0) = g^{00} = 0\,. \tag{E.2}$$

In more physical terms, this implies that characteristic surfaces are locally tangent to light cones as illustrated in Fig. 8. Recalling furthermore that information propagates along characteristics, we also see that information in GR travels along null curves. This is in agreement with our analysis of the linearized Einstein equations where we have seen that the metric perturbations obey the wave equation (B.16).

The null coordinate x^0 is often denoted by u in the literature and we follow this convention here. It is also common to introduce the vector $\boldsymbol{\ell}$ for the normal direction,

$$\boldsymbol{\ell} \coloneqq \mathbf{d}x^0 = \mathbf{d}u\,. \tag{E.3}$$

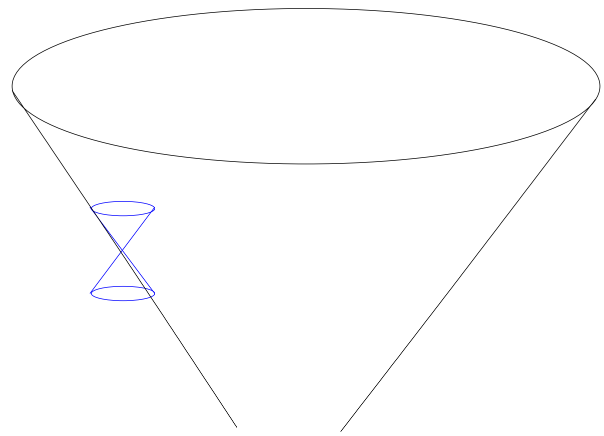


Figure 8: A surface $u = x^0 = \text{const}$ (shown in black) is at any point tangent to the local light cone (displayed in blue).

This completes the first step in our construction of characteristic coordinates: a null coordinate $x^0 = u$ labels three-dimensional null surfaces whose stack constitutes the four-dimensional spacetime manifold. Even without specifying the other coordinates, we can already say quite a lot about the vector $\boldsymbol{\ell}$. First, we find

$$\ell_\alpha = (\mathbf{d}x^0)_\alpha = \delta^0{}_\alpha\,. \tag{E.4}$$

Next, we note that $\boldsymbol{\ell}$ is orthogonal *and* tangent to the null hypersurface $x^0 = \text{const}$,

(i) tangent: $\ell^\alpha(\mathbf{d}x^0)_\alpha = ||\mathbf{d}x^0||^2 = 0\,,$

(ii) orthogonal: $\boldsymbol{\ell} = \mathbf{d}x^0$ is orthogonal to the surface $x^0 = \text{const}$ by construction.

The simultaneous tangent and orthogonal nature of a vector may appear strange at first glance but is typical for null vectors; we are just not used to thinking in terms of null vectors (possibly this was not critical for survival in the stone age...).

The next step in our construction is to look at the integral curves of the vector field ℓ^α. These are curves $x^\alpha(\lambda)$, $\lambda \in \mathbb{R}$ that satisfy the equation

$$\frac{\mathrm{d}x^\alpha}{\mathrm{d}\lambda} = \ell^\alpha = g^{\alpha\mu}\partial_\mu u\,. \tag{E.5}$$

Proposition: The integral curves of ℓ^α are null geodesics and λ is an affine parameter.

Proof. Since partial derivatives commute, we have

$$\partial_\alpha \ell_\beta = \partial_\alpha\partial_\beta u = \partial_\beta \ell_\alpha\,, \tag{E.6}$$

so that

$$\ell^\mu\nabla_\mu\ell_\alpha \;=\; \ell^\mu\nabla_\mu\partial_\alpha u \;=\; \ell^\mu\partial_\mu\partial_\alpha u - \ell^\mu\Gamma^\rho_{\alpha\mu}\partial_\rho u \;=\; \ell^\mu\partial_\alpha\partial_\mu u - \ell^\mu\Gamma^\rho_{\mu\alpha}\partial_\rho u$$

$$= \ell^\mu \nabla_\alpha \ell_\mu = \frac{1}{2}\nabla_\alpha(\ell^\mu \ell_\mu) = 0\,. \tag{E.7}$$

□

So the integral curves of $\boldsymbol{\ell}$ are the curves of propagation of information, i.e. they are the *characteristic curves* or *bicharacteristics* of general relativity.

Def. : A spacetime $(\mathcal{M}, \boldsymbol{g})$ is *asymptotically flat* if there exist Cartesian coordinates such that the metric components $g_{\alpha\beta}$ can be written as

$$g_{\alpha\beta} = \eta_{\alpha\beta} + h_{\alpha\beta}\,,$$

with

$$\lim_{r\to\infty} h_{\alpha\beta} = \mathcal{O}(r^{-1})\,, \qquad \lim_{r\to\infty} \partial_\mu h_{\alpha\beta} = \mathcal{O}(r^{-2})\,, \qquad \lim_{r\to\infty} \partial_\nu \partial_\mu h_{\alpha\beta} \mathcal{O}(r^{-3})\,, \tag{E.8}$$

where $r = \sqrt{x^2 + y^2 + z^2}$ and $\eta_{\alpha\beta}$ is the Minkowski metric in Cartesian coordinates $(t,\, x,\, y,\, z)$.

In asymptotically flat spacetimes, we therefore recover the light cone structure of special relativity at large distance from a radiating source. Let us then consider the 2-dimensional manifold given by constant time and $r \to \infty$. We can label the points on this shell of infinite radius by standard angular coordinates θ, ϕ and integrate from every point the null geodesic equation inwards. This construction of null geodesics and the corresponding choice of the vector field $\boldsymbol{\ell}$ are not unique. This is a consequence of the coordinate freedom of GR; in fact, the set of coordinate transformations which preserve the asymptotic structure of the metric form a symmetry group known as the *Bondi-Metzner-Sachs* or *BMS* group. The BMS group is the generalization of the Lorentz transformations of special relativity for spacetimes that are "only" asymptotically flat. We will employ this coordinate freedom further below to simplify the field equations. For now, the point that matters is that once we have made a choice for the vector field $\boldsymbol{\ell}$, the resulting congruence of null geodesics will fill the characteristic surface without any geodesics crossing at least in some neighbourhood of infinity; cf. Fig. 9. This enables us to construct our characteristic coordinate system as follows.

(1) The null coordinate $x^0 = u$ is chosen such that the surfaces $u =$ const are characteristic surfaces, i.e. such that $g^{00} = 0$.

(2) Defining $\ell_\alpha := (\mathbf{d}u)_\alpha$, the integral curves of ℓ^α are null geodesics, i.e. characteristic curves of GR. We define a radius $x^1 = r$ as a monotonic parameter along each null geodesic.

(3) The angular coordinates θ, ϕ of a point are given by those of the null geodesic that connects the point to infinity.

This coordinate system will break down once null geodesics integrated inwards from $r \to \infty$ cross; we cannot uniquely assign angular coordinates θ, ϕ to such a point of crossing as it connects to infinity through multiple null geodesics. Such a crossing of geodesics will in general

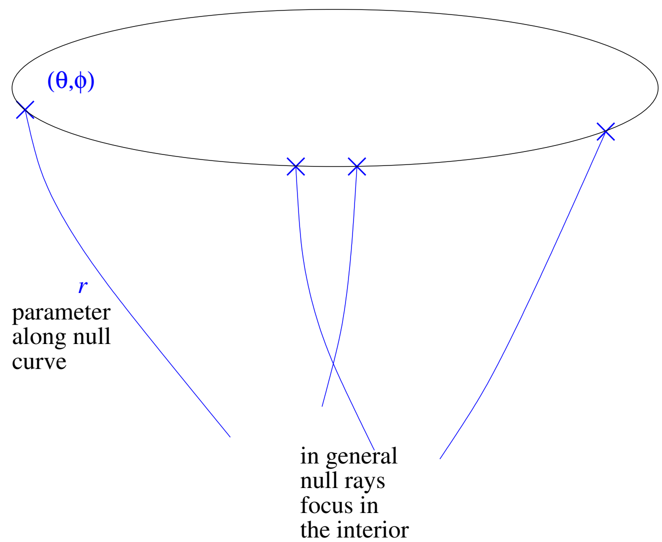


Figure 9: Starting from every point (θ, ϕ) at infinity $r \to \infty$ (black circle), we can integrate the null geodesics inwards (blue curves). In the neighbourhood of infinity the resulting family of null geodesics will fill the characteristic surface without crossing. Further inwards, however, the null geodesics will in general cross due to spacetime curvature, resulting in a breakdown of the characteristic coordinate system.

occur at some sufficiently small radius. This is not a problem, however, since we shall need our characteristic coordinate system only in a neighbourhood of infinity and we can always assume that the interior is modelled using some other coordinate system which we match to the characteristic chart at some sufficiently large radius. This approach forms the core of the Cauchy-characteristic matching technique mentioned above; for more details see [22].

E.2 The Bondi metric

Having established our coordinate system, we next consider the resulting structure of the metric components. In the coordinates $x^\alpha = (u, r, \theta, \phi)$ the tangent vector to the null geodesics is

$$\frac{\mathrm{d}x^\alpha}{\mathrm{d}r} = \delta^\alpha{}_1 \,, \tag{E.9}$$

and it must be proportional to ℓ^α, since the null geodesics are integral curves of $\boldsymbol{\ell}$. This implies

$$\ell^\alpha = \sigma\, \delta^\alpha{}_1 \quad \text{for some} \quad \sigma \in \mathbb{R}\,, \quad \sigma \neq 0\,. \tag{E.10}$$

Here, we impose the condition $\sigma \neq 0$ to ensure that we have a monotonically varying parameter r along the null geodesics. In consequence,

$$\begin{aligned} & \ell^\alpha = g^{\alpha\mu}\partial_\mu u = g^{\alpha\mu}\delta^0{}_\mu = g^{\alpha 0} = g^{0\alpha} \overset{!}{=} \sigma\, \delta^\alpha{}_1 \\ \Rightarrow \quad & g^{00} = g^{02} = g^{03} = 0\,. \end{aligned} \tag{E.11}$$

The inverse metric thus has the form

$$g^{\alpha\beta} = \begin{pmatrix} 0 & \sigma & 0 & 0 \\ \sigma & g^{11} & g^{12} & g^{13} \\ 0 & g^{21} & g^{22} & g^{23} \\ 0 & g^{31} & g^{32} & g^{33} \end{pmatrix} . \tag{E.12}$$

The metric components $g_{\beta\gamma}$ are obtained by inverting the matrix (E.12) which we do by constructing the cofactor matrix $C^{\mu\nu}$. The component $C^{\mu\nu}$ is obtained by crossing out in $g^{\alpha\beta}$ the row μ and the column ν, calculating the determinant of the resulting reduced matrix and finally adjusting by the $+$ or $-$ sign given by the usual $\begin{matrix} + & - \\ - & + \end{matrix}$ pattern in the calculation of determinants. The inverse of $g^{\alpha\beta}$ is then obtained by taking the adjunct of the cofactor matrix $C^{\alpha\beta}$ and dividing by $\det g^{\alpha\beta}$. Consider first, the component C^{11},

$$C^{11} = \begin{vmatrix} 0 & 0 & 0 \\ 0 & g^{22} & g^{23} \\ 0 & g^{32} & g^{33} \end{vmatrix} = 0 \, , \tag{E.13}$$

so that $g_{11} = 0$. We likewise obtain

$$C^{12} = - \begin{vmatrix} 0 & \sigma & 0 \\ 0 & g^{21} & g^{23} \\ 0 & g^{31} & g^{33} \end{vmatrix} = 0 \, , \tag{E.14}$$

and $C^{13} = 0$ in the same way. The metric components in our characteristic coordinate system thus satisfy

$$g_{11} = g_{12} = g_{13} = 0 \, . \tag{E.15}$$

We next fix the radial coordinate r by the requirement that 2-spheres $u = \text{const}$, $r = \text{const}$ have proper area $A = 4\pi r^2$. This radial coordinate is often called the *areal radius* or *luminosity distance parameter*, and the condition implies that (you may wish to check this as an exercise)

$$\begin{vmatrix} g_{22} & g_{23} \\ g_{32} & g_{33} \end{vmatrix} = r^4 \sin^2\theta \, . \tag{E.16}$$

In order to reduce the amount of calculations, we will now restrict ourselves to spacetimes that are axially symmetric and invariant under azimuthal reflection. This is the scenario originally studied by Bondi *et al* [3] and will illustrate the main features of gravitational radiation as derived in non-linear GR. The extension to general spacetimes was derived by Sachs [4] shortly afterwards and we will summarize the resulting changes at the end of our discussion.

Azimuthal reflection symmetry implies that the line element $\mathrm{d}s^2$ is invariant under the change $\mathrm{d}\phi \to -\mathrm{d}\phi$ and thus requires that

$$g_{03} = g_{13} = g_{23} = 0 \, , \tag{E.17}$$

and axial symmetry enables us to construct angular coordinates such that

$$\frac{\partial g_{\alpha\beta}}{\partial\phi} = 0\,. \tag{E.18}$$

Equations (E.15) and (E.17) eliminate 5 of the 10 metric components and the condition (E.16) for the areal radius fixes the product $g_{22}\,g_{33}$, so that we are left with 4 independent components,

$$g_{\alpha\beta} = \begin{pmatrix} g_{00} & g_{01} & g_{02} & 0 \\ g_{01} & 0 & 0 & 0 \\ g_{02} & 0 & g_{22} & 0 \\ 0 & 0 & 0 & r^4\sin^2\theta/g_{22} \end{pmatrix}. \tag{E.19}$$

It turns out convenient to represent the 4 remaining degrees of freedom in terms of four functions V, β, U and γ of (u, r, θ) such that the line element is given by the *Bondi radiation metric*

$$\mathrm{d}s^2 = \left(-\frac{V}{r}e^{2\beta} + U^2r^2e^{2\gamma}\right)\mathrm{d}u^2 - 2e^{2\beta}\mathrm{d}u\,\mathrm{d}r - 2Ur^2e^{2\gamma}\mathrm{d}u\,\mathrm{d}\theta + r^2(e^{2\gamma}\mathrm{d}\theta^2 + e^{-2\gamma}\sin^2\theta\,\mathrm{d}\phi^2)\,. \tag{E.20}$$

In matrix form, this gives us the following.

Proposition: The Bondi metric and its inverse are given by

$$\begin{aligned} g_{\alpha\beta} &= \begin{pmatrix} -\frac{V}{r}e^{2\beta} + r^2U^2e^{2\gamma} & -e^{2\beta} & -r^2Ue^{2\gamma} & 0 \\ -e^{2\beta} & 0 & 0 & 0 \\ -r^2Ue^{2\gamma} & 0 & r^2e^{2\gamma} & 0 \\ 0 & 0 & 0 & r^2e^{-2\gamma}\sin^2\theta \end{pmatrix} \\ g^{\alpha\beta} &= \begin{pmatrix} 0 & -e^{-2\beta} & 0 & 0 \\ -e^{-2\beta} & \frac{V}{r}e^{-2\beta} & -Ue^{-2\beta} & 0 \\ 0 & -Ue^{-2\beta} & r^{-2}e^{-2\gamma} & 0 \\ 0 & 0 & 0 & r^{-2}e^{2\gamma}\sin^{-2}\theta \end{pmatrix}. \end{aligned} \tag{E.21}$$

Proof. We have already derived the covariant metric and only need to compute its inverse. The determinant is given by

$$\det g_{\alpha\beta} = r^2e^{-2\gamma}\sin^2\theta \begin{vmatrix} -\frac{V}{r}e^{2\beta} + r^2U^2e^{2\gamma} & -e^{2\beta} & 0 \\ -e^{2\beta} & 0 & 0 \\ -r^2Ue^{2\gamma} & 0 & r^2e^{2\gamma} \end{vmatrix} = -e^{4\beta}r^4\sin^2\theta\,. \tag{E.22}$$

The rest is a straightforward calculation of the cofactor matrix elements [recall that for $C^{\mu\nu}$ we cross out row μ and column ν in $g_{\alpha\beta}$, compute the determinant of the remainder and multiply with $(-1)^{\mu+\nu}$], whence $g^{\alpha\beta} = C^{\beta\alpha}/\det g_{\mu\nu}$. The complete list of these calculations is as follows.

$$00: \quad C^{00} = 0 \quad \Rightarrow \quad g^{00} = 0\,,$$

$$
\begin{aligned}
01:\quad & C^{01} = -\begin{vmatrix} -e^{2\beta} & 0 & 0 \\ -r^2 U e^{2\gamma} & r^2 e^{2\gamma} & 0 \\ 0 & 0 & r^2 e^{-2\gamma}\sin^2\theta \end{vmatrix} = r^4 e^{2\beta}\sin^2\theta \\
& \Rightarrow g^{10} = -e^{-2\beta} = g^{01}\,, \\
02:\quad & C^{02} = 0 \quad \Rightarrow \quad g^{02} = g^{20} = 0\,, \\
03:\quad & C^{03} = 0 \quad \Rightarrow \quad g^{03} = g^{30} = 0 \\
11:\quad & C^{11} = \begin{vmatrix} -\frac{V}{r}e^{2\beta} + r^2U^2e^{2\gamma} & -r^2Ue^{2\gamma} & 0 \\ -r^2Ue^{2\gamma} & r^2e^{2\gamma} & 0 \\ 0 & 0 & r^2e^{-2\gamma}\sin^2\theta \end{vmatrix} = r^2e^{-2\gamma}\sin^2\theta\left(-rVe^{2\beta+2\gamma}\right) = -r^3Ve^{2\beta}\sin^2\theta \\
& \Rightarrow g^{11} = \frac{C^{11}}{\det g_{\alpha\beta}} = r^{-1}Ve^{-2\beta}\,, \\
12:\quad & C^{12} = -\begin{vmatrix} -\frac{V}{r}e^{2\beta} + r^2U^2e^{2\gamma} & -e^{2\beta} & 0 \\ -r^2Ue^{2\gamma} & 0 & 0 \\ 0 & 0 & r^2e^{-2\gamma}\sin^2\theta \end{vmatrix} = -r^2e^{-2\gamma}\sin^2\theta(-r^2Ue^{2\gamma+2\beta}) = r^4Ue^{2\beta}\sin^2\theta \\
& \Rightarrow g^{21} = -Ue^{-2\beta} = g^{12}\,, \\
13:\quad & C^{13} = 0 \quad \Rightarrow \quad g^{31} = g^{13} = 0\,, \\
22:\quad & C^{22} = \begin{vmatrix} -\frac{V}{r}e^{2\beta} + r^2U^2e^{2\gamma} & -e^{2\beta} & 0 \\ -e^{2\beta} & 0 & 0 \\ 0 & 0 & r^2e^{-2\gamma}\sin^2\theta \end{vmatrix} = -r^2e^{-2\gamma}\sin^2\theta e^{4\beta} \\
& \Rightarrow g^{22} = r^{-2}e^{-2\gamma}\,, \\
23:\quad & C^{23} = 0 \quad \Rightarrow \quad g^{23} = g^{32} = 0\,, \\
33:\quad & C^{33} = -r^2e^{2\gamma}e^{4\beta} \quad \Rightarrow \quad g^{33} = r^{-2}e^{2\gamma}\sin^{-2}\theta\,.
\end{aligned} \tag{E.23}
$$

□

E.3 The characteristic field equations

In principle, we could now plug the Bondi metric (E.21) into the machinery for computing the Ricci tensor and thus write down the vacuum Einstein equations $R_{\alpha\beta} = 0$ as a PDE system for the functions V, U, β and γ. Doing so one finds that the components $R_{03} = R_{13} = R_{23} = 0$ vanish identically. The other components, however, are lengthy and we obtain rather more insight into the Einstein equations by first studying how the contracted Bianchi identities (A.3) relate the remaining components of the Ricci tensor. For this purpose, we write the Bianchi identities as follows.

Lemma :

$$\nabla^\mu G_{\alpha\mu} = g^{\mu\rho}\left(\partial_\rho R_{\alpha\mu} - \Gamma^\sigma_{\mu\rho} R_{\alpha\sigma} - \frac{1}{2}\partial_\alpha R_{\mu\rho}\right) \tag{E.24}$$

Proof.

$$\begin{aligned}
\nabla^\mu G_{\alpha\mu} &= g^{\mu\rho}\nabla_\rho\left(R_{\alpha\mu} - \frac{1}{2}g_{\alpha\mu}R\right) \\
&= g^{\mu\rho}\left(\partial_\rho R_{\alpha\mu} - \Gamma^\sigma_{\alpha\rho}R_{\sigma\mu} - \Gamma^\sigma_{\mu\rho}R_{\alpha\sigma} - \frac{1}{2}g_{\alpha\mu}\partial_\rho R\right) \\
&= g^{\mu\rho}\left(\partial_\rho R_{\alpha\mu} - \Gamma^\sigma_{\mu\rho}R_{\alpha\sigma}\right) - g^{\mu\rho}\Gamma^\sigma_{\alpha\rho}R_{\sigma\mu} - \frac{1}{2}\partial_\alpha(\underbrace{g^{\sigma\tau}R_{\sigma\tau}}_{=g^{\mu\rho}R_{\mu\rho}}) \\
&= g^{\mu\rho}\left(\partial_\rho R_{\alpha\mu} - \Gamma^\sigma_{\mu\rho}R_{\alpha\sigma} - \frac{1}{2}\partial_\alpha R_{\mu\rho}\right) - \left(\frac{1}{2}\partial_\alpha g^{\sigma\mu} + g^{\mu\rho}\Gamma^\sigma_{\alpha\rho}\right)R_{\sigma\mu}
\end{aligned} \tag{E.25}$$

This is the required result provided the second term on the right-hand side vanishes. To show that this is indeed the case, we use the relation

$$g^{\mu\nu}\partial_\alpha g_{\mu\rho} = -g_{\mu\rho}\partial_\alpha g^{\mu\nu}\,. \tag{E.26}$$

Then we obtain

$$\begin{aligned}
\left(\frac{1}{2}\partial_\alpha g^{\sigma\mu} + g^{\mu\rho}\Gamma^\sigma_{\alpha\rho}\right)R_{\sigma\mu} &= \left[\frac{1}{2}\partial_\alpha g^{\sigma\mu} + \frac{1}{2}g^{\mu\rho}g^{\sigma\tau}(-\partial_\tau g_{\alpha\rho} + \partial_\alpha g_{\rho\tau} + \partial_\rho g_{\tau\alpha})\right]R_{\sigma\mu} \\
&= \frac{1}{2}\left[\partial_\alpha g^{\sigma\mu} + g^{\sigma\tau}g_{\alpha\rho}\partial_\tau g^{\mu\rho} - g^{\mu\rho}g_{\rho\tau}\partial_\alpha g^{\sigma\tau} - g^{\mu\rho}g_{\tau\alpha}\partial_\rho g^{\sigma\tau}\right]R_{\sigma\mu} \\
&= \frac{1}{2}\left(g^{\sigma\tau}g_{\alpha\rho}\partial_\tau g^{\mu\rho} - g^{\mu\tau}g_{\rho\alpha}\partial_\tau g^{\sigma\rho}\right)R_{\sigma\mu} = 0\,,
\end{aligned} \tag{E.27}$$

because the expression in parentheses on the last line is asymmetric in (σ, μ) and $R_{\sigma\mu}$ is symmetric. □

We will next look at the individual components of the contracted Bianchi identities in the form (E.24). For this purpose, let us assume that we have solved by some means four of the vacuum Einstein equations, namely the so-called *main equations* $R_{11} = R_{12} = R_{22} = R_{33} = 0$. Furthermore, we recall that the components $R_{03} = R_{13} = R_{23}$ vanish identically and that the inverse Bondi metric is given by (E.21). In summary, this gives us

$$\begin{aligned}
g^{00} = g^{02} = g^{03} &= 0\,, & R_{03} &= 0\,, \\
g^{13} &= 0\,, & R_{11} = R_{12} = R_{13} &= 0\,, \\
g^{20} = g^{23} &= 0\,, & R_{21} = R_{22} = R_{23} &= 0\,,
\end{aligned}$$

$$g^{30} = g^{31} = g^{32} = 0\,, \qquad\qquad R_{30} = R_{31} = R_{32} = R_{33} = 0\,, \tag{E.28}$$

which simplifies our calculation considerably. Expanding Eq. (E.24) then gives us

$$\begin{aligned}
\alpha = 0: \qquad & g^{0\rho}\partial_\rho R_{00} + g^{1\rho}\partial_\rho R_{01} + g^{2\rho}\partial_\rho R_{02} - g^{\mu\rho}\Gamma^0_{\mu\rho}R_{00} - g^{\mu\rho}\Gamma^1_{\mu\rho}R_{01} - g^{\mu\rho}\Gamma^2_{\mu\rho}R_{02} \\
& - \frac{1}{2}g^{01}\partial_0 R_{01} - \frac{1}{2}g^{10}\partial_0 R_{10} = 0 \\
\Rightarrow \quad & g^{01}\partial_1 R_{00} + g^{10}\partial_0 R_{01} + g^{11}\partial_1 R_{01} + g^{12}\partial_2 R_{01} + g^{21}\partial_1 R_{02} + g^{22}\partial_2 R_{02} \\
& - g^{\mu\rho}\Gamma^0_{\mu\rho}R_{00} - g^{\mu\rho}\Gamma^1_{\mu\rho}R_{01} - g^{\mu\rho}\Gamma^2_{\mu\rho}R_{02} - g^{01}\partial_0 R_{01} = 0\,.
\end{aligned} \tag{E.29}$$

$$\begin{aligned}
\alpha = 1: \qquad & g^{\mu\rho}\partial_\rho R_{1\mu} - g^{\mu\rho}\Gamma^\sigma_{\mu\rho}R_{1\sigma} - \frac{1}{2}g^{\mu\rho}\partial_1 R_{\mu\rho} = 0 \\
\Rightarrow \quad & g^{0\rho}\partial_\rho R_{10} - g^{\mu\rho}\Gamma^0_{\mu\rho}R_{10} - \frac{1}{2}g^{01}\partial_1 R_{01} - \frac{1}{2}g^{10}\partial_1 R_{10} = 0 \\
\Rightarrow \quad & g^{01}\partial_1 R_{10} - g^{\mu\rho}\Gamma^0_{\mu\rho}R_{10} - g^{01}\partial_1 R_{01} = 0 \\
\Rightarrow \quad & - g^{\mu\rho}\Gamma^0_{\mu\rho}R_{10} = 0\,.
\end{aligned} \tag{E.30}$$

$$\begin{aligned}
\alpha = 2: \qquad & g^{\mu\rho}\partial_\rho R_{2\mu} - g^{\mu\rho}\Gamma^\sigma_{\mu\rho}R_{2\sigma} - \frac{1}{2}g^{\mu\rho}\partial_2 R_{\mu\rho} = 0 \\
\Rightarrow \quad & g^{0\rho}\partial_\rho R_{20} - g^{\mu\rho}\Gamma^0_{\mu\rho}R_{20} - g^{01}\partial_2 R_{01} = 0 \\
\Rightarrow \quad & g^{01}\partial_1 R_{20} - g^{\mu\rho}\Gamma^0_{\mu\rho}R_{20} - g^{01}\partial_2 R_{01} = 0\,.
\end{aligned} \tag{E.31}$$

The $\alpha = 3$ component vanishes trivially since all $R_{3\mu} = 0$ and none of our functions depend on $x^3 = \phi$ by axisymmetry. The three above expressions may not look all too helpful, but read in the correct order, they greatly simplify. First, we note that a tedious but straightforward calculation gives us

$$g^{\mu\rho}\Gamma^0_{\mu\rho} = \frac{2}{re^{2\beta}}\,, \tag{E.32}$$

so that Eq. (E.30) directly implies $R_{01} = 0$. Using this result together with (E.32) in Eq. (E.31), we find (note that we now start replacing $\partial_0,\ \partial_1,\ \partial_2$ with $\partial_u,\ \partial_r,\ \partial_\theta$)

$$\begin{aligned}
& g^{01}\partial_1 R_{20} - g^{\mu\rho}\Gamma^0_{\mu\rho}R_{20} = 0 \\
\Rightarrow \quad & -e^{-2\beta}\partial_r R_{20} - 2r^{-1}e^{-2\beta}R_{20} = -e^{-2\beta}\left(\partial_r R_{02} + \frac{2}{r}R_{02}\right) = 0 \\
\Rightarrow \quad & -e^{-2\beta}r^{-2}\partial_r(r^2 R_{02}) = 0\,.
\end{aligned} \tag{E.33}$$

So if the main equations hold, we have $\partial_r(r^2 R_{02}) = 0$ and, hence

$$R_{02} = f(u,\theta)r^{-2}\,, \tag{E.34}$$

for some function f. Now, if $f(u,\theta)=0$ for some radius r, then $R_{02}=0$ everywhere. Together with the above $R_{01}=0$, this simplifies Eq. (E.29) to

$$g^{01}\partial_1 R_{00} - g^{\mu\rho}\Gamma^0_{\mu\rho}R_{00} = 0 \quad \Rightarrow \quad -e^{-2\beta}r^{-2}\partial_r(r^2 R_{00}) = 0\,, \tag{E.35}$$

which is the same equation as (E.33) but now for the component R_{00}, so

$$R_{00} = g(u,\theta)r^{-2}\,, \tag{E.36}$$

for some function g. Again, if $g(u,\theta)=0$ at some radius then we have $R_{00}=0$ everywhere. The equations $R_{00}=0$ and $R_{02}=0$ are commonly referred to as the *supplementary equations*. That leaves us with the main equations which after some crunching of terms (I used `Maple` with the `GRTensor` package) can be written in the following form,

$$R_{11} = -2(\partial_r\gamma)^2 + \frac{4}{r}\partial_r\beta = \frac{4}{r}\left[\partial_r\beta - \frac{1}{2}r(\partial_r\gamma)^2\right] = 0\,, \tag{E.37}$$

$$2r^2R_{12} = \partial_r\left[r^4e^{2(\gamma-\beta)}\partial_r U\right] - 2r^2\left[\partial_r\partial_\theta\beta - \partial_r\partial_\theta\gamma + 2\partial_r\gamma\,\partial_\theta\gamma - 2\cot\theta\,\partial_r\gamma - 2\frac{\partial_\theta\beta}{r}\right] = 0\,, \tag{E.38}$$

$$\begin{aligned}
&e^{2(\beta-\gamma)}R_{22} + r^2e^{2\beta}R^3{}_3 \\
&\quad = -2\partial_r V - \frac{r^4}{2}e^{2(\gamma-\beta)}(\partial_r U)^2 + r^2\partial_r\partial_\theta U + r^2\cot\theta\,\partial_r U + 4r(\partial_\theta U + \cot\theta\, U) \\
&\qquad + 2e^{2(\beta-\gamma)}\left[1 + \cot\theta\,(3\partial_\theta\gamma - \partial_\theta\beta) + \partial_\theta^2\gamma - \partial_\theta^2\beta - (\partial_\theta\beta)^2 - 2(\partial_\theta\gamma)^2 + 2\partial_\theta\beta\,\partial_\theta\gamma\right] \\
&\quad = 0\,,
\end{aligned} \tag{E.39}$$

$$\begin{aligned}
-r^2e^{2\beta}R^3{}_3 = {}& e^{2(\beta-\gamma)}\left[-1 - \cot\theta\,(3\partial_\theta\gamma - 2\partial_\theta\beta) - \partial_\theta^2\gamma + 2\partial_\theta\gamma(\partial_\theta\gamma - \partial_\theta\beta)\right] + 2r\partial_r\partial_u(r\gamma) \\
&+ (1 - r\partial_r\gamma)\partial_r V - (r\partial_r^2\gamma + \partial_r\gamma)V - r(1 - r\partial_r\gamma)\partial_\theta U - r^2(\cot\theta - \partial_\theta\gamma)\partial_r U \\
&+ rU(2r\partial_\theta\partial_r\gamma + 2\partial_\theta\gamma + r\cot\theta\,\partial_r\gamma - 3\cot\theta) = 0\,.
\end{aligned} \tag{E.40}$$

Remarkably, this veritable mess contains only one single term involving a u derivative, marked in orange color. The other equations exclusively involve derivatives inside $u=\text{const}$ surfaces. This is one key benefit of using characteristic coordinates.

Let us for the moment not worry about constants of integration; we'll handle them shortly. Given initial data for the function γ on a surface $u=\text{const}$, we can then formally construct a solution to the entire Einstein equations as follows.

(1) γ is given on a hypersurface $u=u_0$.

(2) Then Eq. (E.37) determines β on this hypersurface.

(3) Then Eq. (E.38) determines U on this hypersurface.

(4) Then Eq. (E.39) determines V on this hypersurface.

(5) From Eq. (E.40) we can compute $\partial_u \gamma$ on this hypersurface.

(6) Knowledge of $\partial_u \gamma$ enables us to update γ from the hypersurface $u = u_0$ to the hypersurface $u = u_0 + \mathrm{d}u$.

In spite of the lengthy expressions on the right-hand sides of Eqs. (E.37)-(E.40), the evolution of initial data obeys a remarkably clear and simple hierarchy. This is due to the fact that each consecutive equation in the above list depends on exactly one additional variable as compared to its predecessor. This is the second key benefit of the characteristic formalism.

But now let us return to the important question of the functions of integration. These are functions that depend on (u, θ) but not on r. By inspection, we immediately see the following.

- Equation (E.37) needs one function of integration $H(u, \theta)$ to determine β.
- Equation (E.38) needs one function for the integration of $\partial_r[r^4 e^{2(\gamma-\beta)} \partial_r U]$; we call this function $-6N(u, \theta)$. We then need a second function $L(u, \theta)$ for the integration of U itself.
- Equation (E.39) needs one function for the integration of V; we call this $-2M(u, \theta)$.
- Equation (E.40) determines $\partial_u \gamma$ except for a function of integration that we dub $\partial_u c(u, \theta)$.

We thus have 5 functions of integration in total and, together with the main equations (E.37)-(E.40) they completely determine the evolution of initial data for γ prescribed at $u = u_0$. We physically interpret this situation as follows. Say, we know the state of a physical system on the hypersurface $u = u_0$ which is a light cone opening to the future as graphically illustrated in Fig. 8. If this system is doing anything "new", such as emitting gravitational radiation, then this development must be mathematically encoded in the functions of integration, since these affect the integration along the outgoing null rays. We will see below that the number of *independent* functions of integration can be reduced from 5 to 1, leaving only the so-called *Bondi news function*. The fact that we only have one news function but two degrees of freedom in vacuum GR is merely a consequence of our restriction to axial symmetry; in the generalized characteristic formalism of Sachs [4], the news function is complex in agreement with our expectation of two degrees of freedom.

Our closer analysis of the functions of integration is based on a series expansion of the metric functions in $\frac{1}{r}$. For this purpose, we consider spacetimes that (i) are asymptotically flat in the sense of Eq. (E.8) and (ii) contain no incoming gravitational radiation originating from past null infinity.

The asymptotic flatness condition implies that $\gamma \propto r^{-1}$ at large radius. In the absence of incoming radiation, the coefficients in the series expansion of γ depend only on retarded time[4] $u = t - r$ but not on advanced time $t + r$. We can then expand

$$\gamma = \frac{f(u, \theta)}{r} + \mathcal{O}(r^{-2}),$$

[4] The relation $u = t - r$ is in general only valid in the limit $r \to \infty$.

for some function f. Plugging this expansion for γ into Eq. (E.40) and, in particular, the orange colored term, we see that

$$\partial_u(r\gamma) = \partial_u f(u,\theta) + \mathcal{O}(r^{-1})\,. \tag{E.41}$$

This is exactly the constant of integration we have labeled $\partial_u c(u,\theta)$ in our above list, so that $f(u,\theta) = c(u,\theta)$ and the expansion of γ becomes

$$\gamma = \frac{c(u,\theta)}{r} + \mathcal{O}(r^{-2})\,. \tag{E.42}$$

The series expansions for β, U and V are obtained by inserting (E.42) into the main equations (E.37)-(E.39). We illustrate this procedure by computing the series expansion of β from Eq. (E.37),

$$\begin{aligned}
&\partial_r\beta - \frac{1}{2}r(\partial_r\gamma)^2 = 0 \\
\Rightarrow\quad &\partial_r\beta = \frac{1}{2}r\left[-\frac{c(u,\theta)}{r^2} + \mathcal{O}(r^{-3})\right]^2 = \frac{c(u,\theta)^2}{2r^3} + \mathcal{O}(r^{-4}) \\
\Rightarrow\quad &\beta = H(u,\theta) - \frac{c(u,\theta)^2}{4r^2} + \mathcal{O}(r^{-3})\,,
\end{aligned} \tag{E.43}$$

where in the last line we have recalled the constant of integration H. The expansion for U then follows from inserting Eqs. (E.42) and (E.43) for γ and β into Eq. (E.38) and by substituting for γ, β and U in Eq. (E.39), we obtain the series of V. This calculation becomes quite lengthy and is most conveniently done with a symbolic manipulation tool like `Mathematica` or `Maple`. The result is

$$U = L + 2e^{2H}\partial_\theta H r^{-1} - e^{2H}\left[\partial_\theta c + 2c\partial_\theta H + 2\cot\theta c\right]r^{-2} + \ldots\,, \tag{E.44}$$

$$V = \left[L\cot\theta + \partial_\theta L\right]r^2 + e^{2H}\left[1 - (\partial_\theta H)^2 - \partial_\theta^2 H - \cot\theta\partial_\theta H\right]r + \ldots\,. \tag{E.45}$$

Together with Eqs. (E.42) and (E.43), these are our preliminary series expansions of the metric variables. Next, we will eliminate the functions of integration L and H.

Proposition: For asymptotically flat spacetimes with no gravitational radiation coming in from infinity, the constant of integration L vanishes: $L(u,\theta) = 0$.

Proof. We will show that the assumption $L(u,\theta) \neq 0$ leads to a contradiction. For this purpose, we recall that $\boldsymbol{\partial}_u$ is by construction a time like vector. Using Eqs. (E.44) and (E.45) can be written as

$$\boldsymbol{g}(\boldsymbol{\partial}_u,\boldsymbol{\partial}_u) = g_{00} = -\frac{V}{r}e^{2\beta} + U^2r^2e^{2\gamma} = L^2r^2 + \mathcal{O}(r^1)\,, \tag{E.46}$$

which is manifestly in contradiction to the timelike nature of $\boldsymbol{\partial}_u$. The only way to avoid this contradiction is that $L(u,\theta) = 0$. $\square$

Proposition: We can choose the coordinates (u, r, θ, ϕ) such that the form of the Bondi metric (E.21) is preserved *and* $H(u, \theta) = 0$.

Proof. Let us define new coordinates $\bar{x}^\alpha = (\bar{u}, \bar{r}, \bar{\theta}, \bar{\phi})$ by

$$\begin{aligned} u &= A_0(\bar{u}, \bar{\theta}) + A_1(\bar{u}, \bar{\theta})\bar{r}^{-1} + \dots , \\ r &= \bar{r} + \rho_0(\bar{u}, \bar{\theta}) + \dots , \\ \theta &= \bar{\theta} + B_1(\bar{u}, \bar{\theta})\bar{r}^{-1} + \dots , \end{aligned} \tag{E.47}$$

while $\bar{\phi} = \phi$ remains unchanged. Next, we consider the series expansion in $1/r$ of the metric components which we find by inserting the corresponding expansions (E.42), (E.43) and (E.44) for the functions γ, β and U as well as using $V \sim r$. This gives us

$$\begin{aligned} g_{uu} &= \text{const} + \mathcal{O}(r^{-1}) , \\ g_{ur} &= -e^{2H} + \mathcal{O}(r^{-2}) , \\ g_{u\theta} &= -r^2 U e^{2\gamma} \;=\; -2re^{2H}\partial_\theta H + \mathcal{O}(r^0) , \\ g_{\theta\theta} &= r^2 e^{2\gamma} \;=\; r^2 + 2cr + \mathcal{O}(r^0) , \\ g_{\phi\phi} &= r^2 \sin^2\theta \, e^{-2\gamma} \;=\; r^2 \sin^2\theta - 2cr \sin^2\theta + \mathcal{O}(r^0) . \end{aligned} \tag{E.48}$$

We also recall that $g_{u\phi} = g_{rr} = g_{r\theta} = g_{r\phi} = g_{\theta\phi} = 0$. The metric components then transform according to

$$\bar{g}_{\alpha\beta} = \frac{\partial x^\mu}{\partial \bar{x}^\alpha} \frac{\partial x^\nu}{\partial \bar{x}^\beta} g_{\mu\nu} . \tag{E.49}$$

We thus find

$$\begin{aligned} \bar{g}_{\bar{r}\bar{r}} &= \frac{\partial x^\mu}{\partial \bar{r}} \frac{\partial x^\nu}{\partial \bar{r}} g_{\mu\nu} \;=\; \frac{\partial u}{\partial \bar{r}} \frac{\partial u}{\partial \bar{r}} g_{uu} + 2\frac{\partial u}{\partial \bar{r}} \frac{\partial r}{\partial \bar{r}} g_{ur} + 2\frac{\partial u}{\partial \bar{r}} \frac{\partial \theta}{\partial \bar{r}} g_{u\theta} + \frac{\partial \theta}{\partial \bar{r}} \frac{\partial \theta}{\partial \bar{r}} g_{\theta\theta} \\ &= \left(-\frac{A_1}{\bar{r}^2} + \dots\right)^2 g_{uu} + 2\left(-\frac{A_1}{\bar{r}^2} + \dots\right)(1 + \dots) g_{ur} + 2\left(-\frac{A_1}{\bar{r}^2} + \dots\right)\left(-\frac{B_1}{\bar{r}^2}\right) g_{u\theta} \\ &\quad + \left(-\frac{B_1}{\bar{r}^2} + \dots\right)^2 g_{\theta\theta} \\ &= -\frac{2A_1}{\bar{r}^2}(-e^{2H}) + \frac{B_1^2}{\bar{r}^2} + \mathcal{O}(\bar{r}^{-3}) \;=\; 2A_1 e^{2H} \bar{r}^{-2} + B_1^2 \bar{r}^{-2} + \mathcal{O}(\bar{r}^{-3}) , \\ \bar{g}_{\bar{r}\bar{\theta}} &= \frac{\partial r}{\partial \bar{r}} \frac{\partial u}{\partial \bar{\theta}} g_{ur} + \frac{\partial \theta}{\partial \bar{r}} \frac{\partial \theta}{\partial \bar{\theta}} g_{\theta\theta} + \mathcal{O}(\bar{r}^{-1}) \end{aligned}$$

$$
\begin{aligned}
&= -e^{2H}\partial_{\bar\theta}A_0 - B_1 + \mathcal{O}(r^{-1})\,, \\
\bar g_{\bar\theta\bar\theta} &= 2\frac{\partial u}{\partial\bar\theta}\frac{\partial\theta}{\partial\bar\theta}g_{u\theta} + \frac{\partial\theta}{\partial\bar\theta}\frac{\partial\theta}{\partial\bar\theta}g_{\theta\theta} + \mathcal{O}(r^0) \\
&= 2\partial_{\bar\theta}A_0(-2r\partial_\theta H\, e^{2H}) + (1+\partial_{\bar\theta}B_1\bar r^{-1})^2(r^2+2rc) + \mathcal{O}(\bar r^0) \\
&= 2\partial_{\bar\theta}A_0(-2r\partial_\theta H\, e^{2H}) + (1+\partial_{\bar\theta}B_1\bar r^{-1})^2[(\bar r+\rho_0)^2+2c\bar r] + \mathcal{O}(\bar r^0) \\
&= \bar r^2 + 2c\bar r + 2\rho_0\bar r + 2\partial_{\bar\theta}B_1\bar r - 4\partial_{\bar\theta}A_0\partial_\theta H e^{2H}\bar r + \mathcal{O}(\bar r^0) \\
\bar g_{\bar\phi\bar\phi} &= r^2\sin^2\theta e^{-2\gamma} \quad = \quad (\bar r+\rho_0)^2\sin^2(\bar\theta + B_1\bar r^{-1}) - 2c\bar r\sin^2\bar\theta + \mathcal{O}(\bar r^0) \\
&= \bar r^2(\sin\bar\theta + B_1\bar r^{-1}\cos\bar\theta)^2 + 2\rho_0\bar r\sin^2\bar\theta - 2c\bar r\sin^2\bar\theta + \mathcal{O}(\bar r^0) \\
&= \bar r^2\sin^2\bar\theta + 2B_1\bar r\sin^2\bar\theta\cot\bar\theta + 2\rho_0\bar r\sin^2\bar\theta - 2c\sin^2\bar\theta\,\bar r + \mathcal{O}(\bar r^0) \\
&= \sin^2\bar\theta\left(\bar r^2 + 2\bar r\rho_0 + 2\bar r B_1\cot\bar\theta - 2c\bar r\right) + \mathcal{O}(\bar r^0)\,, \\
g_{\bar u\bar r} &= \frac{\partial u}{\partial\bar u}\frac{\partial r}{\partial\bar r}g_{ur} + \mathcal{O}(\bar r^{-1}) \\
&= -e^{2H}\partial_{\bar u}A_0 + \mathcal{O}(\bar r^{-1})\,.\,. \qquad \text{(E.50)}
\end{aligned}
$$

For the product $g_{\bar\theta\bar\theta}g_{\bar\phi\bar\phi}$ we find

$$
\begin{aligned}
g_{\bar\theta\bar\theta}g_{\bar\phi\bar\phi} &= \bar r^2\left[1 + 2\frac{c}{\bar r} + 2\frac{\rho_0}{\bar r} + 2\partial_{\bar\theta}B_1\frac{1}{\bar r} - 4\frac{\partial_{\bar\theta}A_0}{\bar r}\partial_\theta H e^{2H}\right] \\
&\quad\times\bar r^2\sin^2\bar\theta\left[1 + 2\frac{\rho_0}{\bar r} + 2\frac{B_1}{\bar r}\cot\bar\theta - 2\frac{c}{\bar r}\right] + \mathcal{O}(\bar r^2) \\
&= \bar r^4\sin^2\bar\theta\left[1 + 4\frac{\rho_0}{\bar r} + 2\frac{\partial_{\bar\theta}B_1}{\bar r} + \frac{2}{\bar r}B_1\cot\bar\theta - 4\frac{\partial_{\bar\theta}A_0}{\bar r}\partial_\theta H e^{2H}\right]\,. \qquad \text{(E.51)}
\end{aligned}
$$

Requiring $g_{\bar r\bar r} = g_{\bar r\bar\theta} = 0$ and $g_{\bar\theta\bar\theta}g_{\bar\phi\bar\phi} = \bar r^4\sin^2\bar\theta$ then implies at leading order

$$
\begin{aligned}
&2A_1e^{2H} = -B_1^2\,, \\
&B_1 = -e^{2H}\partial_{\bar\theta}A_0\,, \\
&2\rho_0 + \partial_{\bar\theta}B_1 + B_1\cot\theta - 2\partial_{\bar\theta}A_0\,\partial_\theta H e^{2H} = 0\,. \qquad \text{(E.52)}
\end{aligned}
$$

In Eq. (E.50) we can thus choose $\partial_{\bar u}A_0 = e^{-2H}$ so that $g_{\bar u\bar r} = -1$ and $H = 0$ in our new coordinate system. The second equation in (E.52) then determines B_1 in terms of A_0, the first equation determines A_1 and the third determines ρ_0. Likewise, the higher-order terms in these equations determine the higher-order coefficients in the coordinate transformation (E.47). □

Now that we have shown the vanishing of the the two functions of integration, $L(u,\theta) = 0 = H(u,\theta)$, it is a good time to review our expansion and also add a few higher-order terms. We recall that the metric is given by Eq. (E.21) and the functions satisfy the main equations (E.37)-(E.40). The starting point to explore the series expansions is the outgoing radiation condition (E.41). We have already seen that the function f in that equation equals the function of integration c. We furthermore extend the series expansion of γ to the order r^{-3}. Inserting this expansion into Eqs. (E.38) and (E.39) for β and U, a straightforward calculation shows that the $\sim r^{-2}$ in the expansion of γ leads to logarithmic terms $\ln r$ in the expansion of U which, ultimately, can be shown to contradict the outgoing radiation condition of the other metric variables. We do not consider such potentially problematic spacetimes and therefore assume that γ contain no $\sim r^{-2}$ term,

$$\gamma(u,r,\theta) = c(u,\theta)r^{-1} + \left[e(u,\theta) - \frac{1}{6}c(u,\theta)^3\right] r^{-3} + \mathcal{O}(r^{-4})\,, \tag{E.53}$$

where we have followed Bondi's [3] notation for the $\sim r^{-3}$ coefficient. Inserting this into Eq. (E.38) gives us the expansion for β (recall that the function of integration H vanishes),

$$\beta = -\frac{1}{4}c^2 r^{-2} + \left[\frac{c^4}{8} - \frac{3}{4}ce\right] r^{-4} + \mathcal{O}(r^{-6})\,, \tag{E.54}$$

Inserting both γ and β into Eq. (E.38) gives us the expansion for U (recall that the function of integration L vanishes),

$$\begin{aligned} U &= \left[-\partial_\theta c - 2c\cot\theta\right] r^{-2} + \left[2N + \frac{4}{3}c\partial_\theta c + \frac{8}{3}c^2\cot\theta\right] r^{-3} \\ &\quad + \left[-2c^3\cot\theta + 3e\cot\theta - \frac{3}{2}c^2\partial_\theta c - 3Nc + \frac{3}{2}\partial_\theta e\right] r^{-4} + \mathcal{O}(r^{-5})\,. \end{aligned} \tag{E.55}$$

Note that our coefficients for r^{-3} and r^{-4} differ slightly from Eq. (32) in Bondi's work [3]. Despite careful checks of our results, including a calculation with `Maple`, we cannot rule out an error on our side. These higher-order terms have no impact on our conclusions, however, and we mention this discrepancy here for completeness only.

The final step consists in using the expansions for γ, β and U in Eq. (E.39) which gives us the expansion for V,

$$
\begin{aligned}
V \;=\;& r - 2M \\
&+ \left[\frac{37}{6} c\partial_\theta c \cot\theta - N\cot\theta + 4c^2\cot^2\theta + \frac{5}{6}c\partial_\theta^2 c - \partial_\theta N - \frac{c^2}{6} + \frac{11}{6}(\partial_\theta c)^2\right] r^{-1} \\
&+ \left[e - \left(6Nc + 5c^2\partial_\theta c + \frac{3}{2}\partial_\theta e\right)\cot\theta - \frac{3}{2}c(\partial_\theta c)^2 - 4c^3\cot^2\theta - 3N\partial_\theta c - \frac{1}{2}\partial_\theta^2 e\right] r^{-2} \\
&+ \mathcal{O}(r^{-3})\,. \qquad \text{(E.56)}
\end{aligned}
$$

With these expansions in place, we are ready for the final step in reducing the number of independent functions of integration. We still have three such functions, c, M and N. These are related, however, by the supplementary equations $R_{00} = R_{02} = 0$. As we have seen in the discussion around Eqs. (E.34) and (E.36), the sole surviving terms in a series expansion of the supplementary equations are those $\sim r^{-2}$; the vanishing of the corresponding coefficients then provide us with two equations relating c, M and N. **Health warning:** Performing the following calculations without a symbolic computation program like `Maple` or `Mathematica` can have damaging consequences for your mental health.

Expressed in terms of the metric variables, the supplementary equations are very lengthy. Abbreviating $f_u \coloneqq \partial_u f$, $f_r \coloneqq \partial_r f$, $f_{u\theta} = \partial_\theta\partial_u f$ etc. for $f = \gamma,\ \beta,\ U,\ V$, we obtain

$$
\begin{aligned}
R_{00} \;=\;& 2\frac{V}{r}\beta_{ur} - \frac{VV_{rr}}{2r^2} - \frac{V^2\beta_{rr}}{r^2} - \frac{V^2\beta_r}{r^3} - \frac{VV_r\beta_r}{r^2} - \frac{V_u - 2V\beta_u}{r^2} \\
&+\frac{2\beta_{r\theta}UV + \beta_\theta U_r V + \beta_r U_\theta V + 2\beta_r U V_\theta}{r} + \frac{2\beta_\theta UV}{r^2} - \frac{U_\theta V}{2r^2} + \frac{U_\theta V_r}{2r} - \frac{2UV_\theta}{r^2} - \frac{U_r V_\theta}{2r} \\
&-\frac{2\gamma_r U V_\theta}{r} - 2\beta_{ur}U - 2\beta_u U_2 + 2\gamma_{u\theta}U + 2\gamma_u U_\theta + U_{u\theta} + UU_{\theta\theta} + U_\theta^2 \\
&+2(\gamma_\theta - \beta_\theta)UU_\theta + \frac{UV_{r\theta}}{r} + (2\beta_\theta^2 - 2\beta_\theta\gamma_\theta + \gamma_{\theta\theta})U^2 + 2\gamma_u^2 \\
&-\cot\theta\left(2\beta_u U - 2\gamma_u U - U_u - UU_\theta - \gamma_\theta U^2 + \frac{UV}{2r^2} - \frac{UV_r}{2r} - \frac{\beta_r UV}{r}\right) \\
&+r^2 e^{2(\gamma-\beta)}\left[-UU_{ur} - 2\left(\gamma_{ur} + \frac{\gamma_u}{r}\right)U^2 - 2(\gamma_u - \beta_u)UU_r - 2U^2U_{r\theta} - 2UU_rU_\theta\right. \\
&-2\gamma_{r\theta}U^3 - \frac{2}{r}\gamma_\theta U^3 - 3\gamma_\theta U^2 U_r + 2\beta_\theta U^2 U_r + \frac{UU_{rr}V}{r} + \frac{4UU_rV}{r^2} \\
&+2(\gamma_r - \beta_r)\frac{UU_rV}{r} + \frac{\gamma_{rr}U^2V}{r} + \frac{\gamma_r U^2 V}{r} + \frac{\gamma_r U^2 V}{r^2} - \frac{3U^2U_\theta}{r} - \gamma_r U^2 U_\theta \\
&\left.+\frac{U^2V_r}{r^2} + \frac{U_r^2 V}{2r} - U^2\left(U_r + \frac{U}{r} + \gamma_r U\right)\cot\theta\right] + \frac{1}{2}r^4 e^{4(\gamma-\beta)}U^2U_r^2 \\
&-\frac{1}{2r^3}e^{2(\gamma-\beta)}\left[V_{rr} + 2\beta_{rr}V + (2\beta_r - 2\gamma_r + \cot\theta)(V_\theta + 2\beta_\theta V)\right] = 0\,, \qquad \text{(E.57)}
\end{aligned}
$$

$$
\begin{aligned}
R_{02} \;=\;& \beta_{u\theta} - \gamma_{u\theta} + 2\gamma_u\gamma_\theta - 2\gamma_u\cot\theta - U(\beta_{\theta\theta} + 2\beta_\theta^2 - 2\beta_\theta\gamma_\theta + \beta_\theta\cot\theta) \\
&-\frac{V_{r\theta}}{2r} + \frac{V_\theta}{2r^2} + (\gamma_r - \beta_r)\frac{V_\theta}{r} + r^2 e^{2(\gamma-\beta)}\left[\frac{3}{2}UU_{r\theta} + \frac{3UU_\theta}{r} + 2U\left(\gamma_{ur} + \frac{\gamma_u}{r}\right) + \frac{1}{2}U_{ur}\right. \\
&2\gamma_{r\theta}U^2 + (\gamma_u\beta_u)U_r + \gamma_r UU_\theta + (2\gamma_\theta - \beta_\theta)UU_r + U_rU_\theta - \frac{U_{rr}V}{2r} - \frac{UV_r + 2U_rV}{r^2} \\
&-\frac{\gamma_{rr}UV + (\gamma_r - \beta_r)U_rV + \gamma_r UV_r}{r} - \frac{\gamma_r UV}{r^2} + \frac{2\gamma_\theta U^2}{r} \\
&\left.+U\left(\frac{1}{2}U_r + \frac{U}{r} + \gamma_r U\right)\cot\theta\right] - \frac{1}{2}r^4 e^{4(\gamma-\beta)}UU_r^2 = 0\,. \qquad \text{(E.58)}
\end{aligned}
$$

Note that we differ in the 2nd term on the 2nd line of Eq. (E.57) from Bondi's equation in Appendix 2 of Ref. [3] where we have a $\beta_\theta U_r V$ instead of their $\beta_\theta UV_r$. Again, we cannot rule out an error on either behalf. At order r^{-2}, the series expansion of these two equations gives us the relations

$$\partial_u M = -\partial_u c + \frac{1}{2}\partial_\theta^2 \partial_u c + \frac{3}{2}\cot\theta\,\partial_\theta\partial_u c - (\partial_u c)^2\,, \tag{E.59}$$

$$3\partial_u N = -\partial_\theta M - \frac{1}{2}c\partial_\theta\partial_u c + \frac{3}{2}\partial_\theta\partial_u c\,. \tag{E.60}$$

The first of these equations is Bondi's Eq. (35) while the second is similar to Bondi's (36) but differs in some coefficients on the right-hand side. The key point of these equations, however, remains unaffected: If M and N are specified on some initial hypersurface $u = \text{const}$ and c is specified as a function of (u, θ), then the entire evolution of the characteristic field equations is fully determined by the single function c.

E.4 Interpretation of the functions of integration

We can acquire some understanding of the physical significance of the functions of integration by comparing the Bondi metric with specific, analytically known spacetimes. Let us consider for this purpose the Schwarzschild metric

$$\mathrm{d}s^2 = -\left(1 - \frac{2M_\mathrm{S}}{r}\right)\mathrm{d}t^2 + \left(1 - \frac{2M_\mathrm{S}}{r}\right)^{-1}\mathrm{d}r^2 + r^2(\mathrm{d}\theta^2 + \sin^2\theta\,\mathrm{d}\phi^2)\,, \tag{E.61}$$

in outgoing Eddington Finkelstein coordinates. These are given by

$$\tilde{t} = t - 2M_\mathrm{S}\ln|r - 2M_\mathrm{S}|\,, \tag{E.62}$$

and are translated into characteristic coordinates of the Bondi type by defining $u = \tilde{t} - r$. The line element is then given by

$$\mathrm{d}s^2 = -\left(1 - \frac{2M_\mathrm{S}}{r}\right)\mathrm{d}u^2 - 2\mathrm{d}u\mathrm{d}r + r^2(\mathrm{d}\theta^2 + \sin^2\theta\,\mathrm{d}\phi^2)\,, \tag{E.63}$$

which corresponds to the Bondi metric (E.21) for the special case $\gamma = \beta = U = 0$ and $V = r - 2M_\mathrm{S}$. Comparing with the series expansion (E.56) for V, we directly see that for spherically symmetric spacetimes, the function of integration equals the Schwarzschild mass of the spacetime or, equivalently, the Arnowitt-Deser-Misner (ADM) mass [5]. Note that M is indeed constant by virtue of Eq. (E.59) and the vanishing of c.

Bondi *et al* extend this comparison to general axially symmetric static spacetimes which can be written in cylindrical coordinates in the form of the Weyl metric

$$\mathrm{d}s^2 = -e^{2\psi}\mathrm{d}t^2 + e^{-2\psi}\left[e^{2\sigma}(\mathrm{d}\rho^2 + \mathrm{d}z^2) + \rho^2\mathrm{d}\phi^2\right]\,, \tag{E.64}$$

where ψ and σ are functions of ρ and z. The field equations lead to a Laplace equation for ψ,

$$\partial_\rho^2\psi + \frac{1}{\rho}\partial_\rho\psi + \partial_z^2\psi = 0\,, \tag{E.65}$$

and an equation that determines σ in terms of ψ but which we do not require. The solutions ψ for asymptotically flat spacetimes can be expanded in Legendre polynomials and is

$$\psi = \sum_{n=0}^{\infty} A_n R^{-n-1} P_n(\cos\Theta)\,, \tag{E.66}$$

with $\rho = R\sin\Theta$ and $z = R\cos\Theta$. The leading coefficients in this expansion represent the mass m, the dipole D and the quadrupole moment Q according to

$$A_0 = m\,, \qquad A_1 = D\,, \qquad A_2 = Q + \frac{1}{3}m^3\,. \tag{E.67}$$

The coordinate transformation between Weyl and Bondi coordinates is rather tedious and we only quote here the results. In this case, the function c can be written in terms of a transformation function $\alpha(\theta)$,

$$c = -\frac{1}{2}\partial_\theta^2\alpha + \frac{1}{2}\partial_\theta\alpha\cot\theta\,, \tag{E.68}$$

and one then obtains

$$M = m\,, \qquad N = D\sin\theta - m\partial_\theta\alpha\,, \qquad e = \frac{1}{2}Q\sin^2\theta - \partial_\theta\alpha D\sin\theta + \frac{1}{2}m(\partial_\theta\alpha)^2\,, \tag{E.69}$$

where e is the third-order term in the expansion (E.53) of γ. We thus recover the above interpretation of M as the mass of the spacetime while the function N and e are related to the dipole and quadrupole moment of the spacetime; for more details of this calculation see Ref. [3].

The function M is sometimes called the *mass aspect*, and the above result shows that for spherically symmetric spacetimes it equals the mass of the system. In general, however, it will be a function of (u,θ) and we define the mass $m(u)$ as the angle averaged integral

$$m(u) = \frac{1}{4\pi}\int_0^\pi\int_0^{2\pi} M\sin\theta\mathrm{d}\phi\mathrm{d}\theta = \frac{1}{2}\int_0^\pi M(u,\theta)\sin\theta\mathrm{d}\theta\,, \tag{E.70}$$

where the second equality holds for our axisymmetric case. This recovers the limit $m = M$ in spherical symmetry where $M(u,\theta) = \text{const}$, but we can obtain an even more profound result by relating the rate of change of the mass to the news function c via Eq. (E.59). This derivation requires the following Lemma.

Lemma : For axisymmetric spacetimes with no conical singularity on the polar axis, the news function satisfies

$$\lim_{\theta\to 0} c = \lim_{\theta\to\pi} c = 0\,. \tag{E.71}$$

Proof. Let us consider spheres of constant u and r and, more specifically, circles with small constant $\theta = \Delta\theta$. Along these circles, the proper length follows from the Bondi metric (E.21) with $\mathrm{d}u = \mathrm{d}r = \mathrm{d}\theta = 0$,

$$\mathrm{d}s^2 = r^2 e^{-2\gamma}\sin^2\theta\mathrm{d}\phi\,. \tag{E.72}$$

Considering large (but finite) radii, we can expand γ in r^{-1} according to Eq. (E.53). Finally, close to the North pole, $\sin\Delta\theta \approx \Delta\theta$ for small $\Delta\theta$, so that the circumference is

$$l = \int_0^{2\pi} \mathrm{d}s = \int_0^{2\pi} r\sin\Delta\theta e^{-\gamma}\mathrm{d}\phi \approx 2\pi r\Delta\theta\left(1-\frac{c}{r}\right)\,. \tag{E.73}$$

We similarly obtain the proper radius as the integral of $\mathrm{d}s$ from 0 to $\Delta\theta$ along the curve $\mathrm{d}u = \mathrm{d}r = \mathrm{d}\phi = 0$,

$$\rho = \int_0^{\Delta\theta} re^{\gamma}\mathrm{d}\theta \approx r\Delta\theta\left(1+\frac{c}{r}\right)\,. \tag{E.74}$$

In the absence of a conical singularity, the ratio l/ρ must be 2π, so that

$$\frac{l}{\rho} = 2\pi\frac{1-\frac{c}{r}}{1+\frac{c}{r}} \approx 2\pi\left(1-\frac{2c}{r}\right) \stackrel{!}{=} 2\pi\,. \tag{E.75}$$

This is realized only if $\lim_{\theta\to 0} c = 0$. Around the South pole $\theta\to\pi$, we have $\sin(\pi-\Delta\theta)\approx \sin\Delta\theta$ for small $\Delta\theta$ and thus obtain the same expression for l. The integration for ρ now proceeds in the inverse θ direction, so that we use $-\mathrm{d}\theta$ instead of $\mathrm{d}\theta$ and thus also recover the above result (E.74). Again, the ratio $l/\rho = 2\pi$ requires $\lim_{\theta\to\pi} c = 0$. $\square$

With this result under our belt, we are ready to compute the rate of change of the mass $m(u)$.

Proposition: The time evolution of the Bondi mass is given by

$$\partial_u m = -\frac{1}{2}\int_0^{\pi}(\partial_u c)^2\sin\theta\mathrm{d}\theta\,. \tag{E.76}$$

Note that the right-hand side is manifestly non-positive, so m remains constant or decreases. As we will show further below, a non-zero integrand corresponds to emission of gravitational waves.

Proof. Taking the u derivative of Eq. (E.70) and substituting for $\partial_u M$ with the right-hand side of Eq. (E.59) gives us

$$\partial_u m = \frac{1}{2}\int_0^{\pi}\partial_u M\sin\theta\mathrm{d}\theta = -\frac{1}{2}\int_0^{\pi}(\partial_u c)^2\sin\theta\mathrm{d}\theta + \frac{1}{4}\partial_u \underbrace{\int_0^{\pi}\left[-2c+\partial_\theta^2 c + 3\cot\theta\partial_\theta c\right]\sin\theta\mathrm{d}\theta}_{=:I}\,.$$

Splitting the three contributions of $I = I_1 + I_2 + I_3$ in that order, we find through integration by parts ($\int f'g = [fg] - \int fg'$) that

$$I_1 = -2\int_0^{\pi} c\sin\theta\mathrm{d}\theta\,, \tag{E.77}$$

$$I_2 = \int_0^{\pi}\partial_\theta^2 c\,\sin\theta = [\partial_\theta c\,\sin\theta]_0^{\pi} - \int_0^{\pi}\partial_\theta c\,\cos\theta\mathrm{d}\theta$$

$$= \quad 0 - [c\,\cos\theta]_0^\pi + \int_0^\pi c\,(-\sin\theta)\mathrm{d}\theta \quad = \quad -\int_0^\pi c\,\sin\theta\mathrm{d}\theta - [c\,\cos\theta]_0^\pi\,, \tag{E.78}$$

$$I_3 \quad = \quad \int_0^\theta 3\partial_\theta c\,\cos\theta\mathrm{d}\theta \quad = \quad [3c\,\cos\theta]_0^\pi + \int_0^\pi 3c\,\sin\theta\mathrm{d}\theta\,. \tag{E.79}$$

So $I_1 + I_2 + I_3 = [2c\,\cos\theta]_0^\pi$ which vanishes thanks to the Lemma (E.71). □

From our point of view, the most important diagnostic of the characteristic formalism is the GW signal and its relation to the news function. As we have already indicated in Sec. B.3, the relation between the GW polarization modes h_+ and $h_\times$ is most conveniently established by computing the components of the Riemann tensor. For this purpose, however, we first need to relate the characteristic coordinates to those used in the linearized formalism. This task is greatly simplified by the fact that the Riemann tensor is already a perturbative quantity [cf. Eq. (B.6)], so that it will be sufficient to relate the coordinates and their associated unit vectors at background or zeroth-order level.

For this purpose, we first investigate a simpler scenario, the relation of the coordinate vectors in Minkowski spacetime at constant angular position or, equivalently, for the case of two dimensions spanned by the coordinates T and R. The line element in this case is simply

$$\mathrm{d}s^2 = g_{\tilde{\alpha}\tilde{\beta}}\mathrm{d}x^{\tilde{\alpha}}\mathrm{d}x^{\tilde{\beta}} = -\mathrm{d}T^2 + \mathrm{d}R^2\,, \tag{E.80}$$

where the indices $\tilde{\alpha}$, $\tilde{\beta}$ run from 0 to 1. Note that the coordinate vector $\boldsymbol{\partial}_T$ is defined as the tangent vector to the curves $R = \text{const}$ and $\boldsymbol{\partial}_R$ is the coordinate vector tangent to the curves $T = \text{const}$. Both are unit vectors since $\boldsymbol{g}(\boldsymbol{\partial}_T, \boldsymbol{\partial}_T) = -1$ and $\boldsymbol{g}(\boldsymbol{\partial}_R, \boldsymbol{\partial}_R) = 1$. The coordinates and vectors are graphically illustrated in Fig. 10. Next, we define the characteristic coordinates u and r by

$$\begin{array}{ccc} u = T - R & & T = u + r \\ & \Leftrightarrow & \\ r = R & & R = r \end{array}\,. \tag{E.81}$$

Chain rule gives us the characteristic coordinate vectors as

$$\begin{array}{ccc} \boldsymbol{\partial}_u = \dfrac{\partial T}{\partial u}\boldsymbol{\partial}_T + \dfrac{\partial R}{\partial u}\boldsymbol{\partial}_R = \boldsymbol{\partial}_T & & \boldsymbol{\partial}_T = \boldsymbol{\partial}_u \\ & \Leftrightarrow & \\ \boldsymbol{\partial}_r = \dfrac{\partial T}{\partial r}\boldsymbol{\partial}_T + \dfrac{\partial R}{\partial r}\boldsymbol{\partial}_R = \boldsymbol{\partial}_T + \boldsymbol{\partial}_R & & \boldsymbol{\partial}_R = \boldsymbol{\partial}_r - \boldsymbol{\partial}_u \end{array}\,. \tag{E.82}$$

Second, we need to relate the Cartesian directions (x, y, z) used in the linearized approximation to the directions associated with the spherical coordinates (r, θ, ϕ) in the characteristic formalism. This relation is highly non-trivial in general, but becomes relatively simple at infinity where the Bondi metric approaches Minkowski and outgoing GWs become plane waves propagating in the radial direction. At a given point, we can then rotate the Cartesian coordinate system such that the z direction points radially outward, the x direction coincides with that of the polar angle θ and the y direction points in the direction of increasing azimuthal angle ϕ; cf. Fig. 11. At this point, we can identify the unit vectors

$$\mathbf{e}_z = \mathbf{e}_R = -\boldsymbol{\partial}_u + \boldsymbol{\partial}_r\,, \tag{E.83}$$

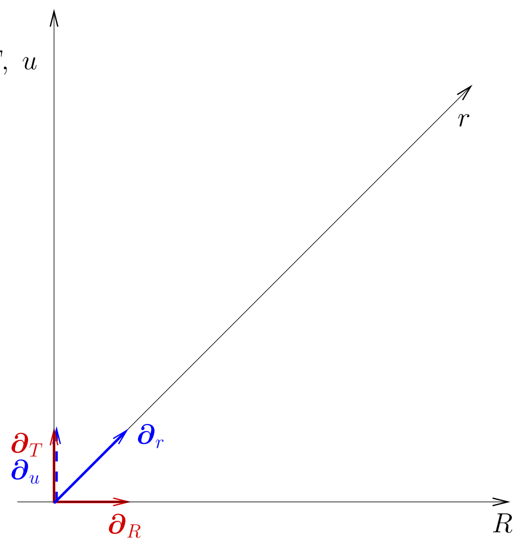


Figure 10: Illustration of the coordinate vectors for the two-dimensional Minkowski spacetime using space-time coordinates (T, R) and for characteristic coordinates (u, r).

$$\mathbf{e}_x = \mathbf{e}_\theta = \frac{1}{r}\boldsymbol{\partial}_\theta \,, \tag{E.84}$$

$$\mathbf{e}_y = \mathbf{e}_\phi = \frac{1}{r\sin\theta}\boldsymbol{\partial}_\phi \,, \tag{E.85}$$

$$\mathbf{e}_T = \mathbf{e}_u = \boldsymbol{\partial}_u \,, \tag{E.86}$$

where the factors in front of the angular coordinate vectors arise from normalization and we have used the above relations (E.82) for the radial coordinate vector $\boldsymbol{\partial}_R$ and the timelike vector $\boldsymbol{\partial}_T$. These relations enable us to compute the components of the Riemann tensor in the linearized regime from the Riemann tensor of the Bondi metric for the limit $r \to \infty$ according to

$$R_{xTxT} = \boldsymbol{R}(\mathbf{e}_x, \mathbf{e}_T, \mathbf{e}_x, \mathbf{e}_T) \,, \tag{E.87}$$

and so on. In the axisymmetric case, 8 of the 20 independent components vanish, leaving us with the 12 independent components

$$\begin{aligned}
&R_{xTxT} = -R_{yTyT} = -R_{xzxT} = R_{yzyT} = R_{xzxz} = -R_{yzyz} = -\partial_u^2 c r^{-1} + \mathcal{O}(r^{-2}) \,, \\
&R_{zTxT} = -R_{zTxz} = -R_{yxyT} = R_{yxyz} = -\left(\partial_\theta\partial_u c + 2\cot\theta\,\partial_u c\right) r^{-2} + \mathcal{O}(r^{-3}) \,, \\
&R_{z0z0} = -R_{xyxy} = -(2M + 2c\partial_u c) r^{-3} + \mathcal{O}(r^{-4}) \,.
\end{aligned} \tag{E.88}$$

The corresponding result obtained in the TT gauge of the linearized regime for a plane wave propagating in the z direction is given by Eq. (B.6) with $h_{\alpha\beta} = H_{\alpha\beta} e^{\mathrm{i}k_\rho x^\rho}$ and $H_{\alpha\beta}$ given by Eq. (B.21). We have used these relations to compute the Riemann components (B.27) needed

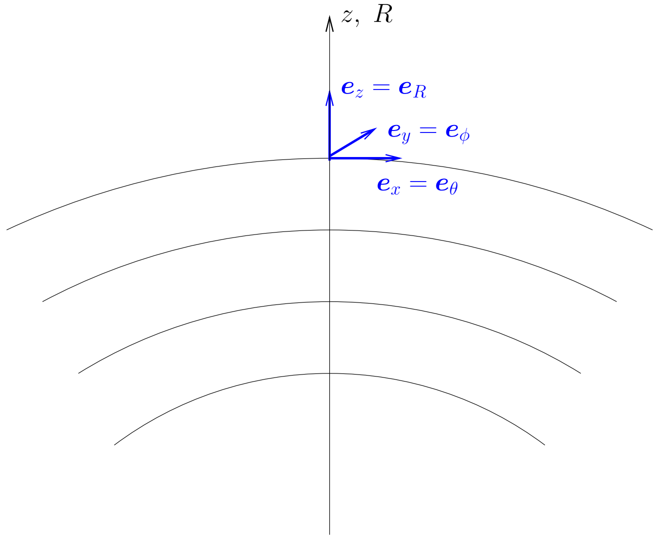


Figure 11: A gravitational wave propagating radially outward. We rotate the Cartesian coordinate system such that the z axis points in the outward radial direction and the polar angle θ points in the x direction. The azimuthal angle ϕ then points in the y direction (into the plane in this figure). Note that the (spatial) outward radial direction is ∂_R whereas ∂_r is a null vector. In the limit of infinite radius, the outgoing wave becomes planar.

for geodesic deviation. The extra components we need here are obtained in a similar fashion, using $h_{z\alpha} = 0$ and the fact that for an outgoing wave

$$h_{\alpha\beta} = f(t - z) \qquad \Rightarrow \qquad \partial_z h_{\alpha\beta} = -\partial_0 h_{\alpha\beta}\,. \tag{E.89}$$

Close inspection of the perturbative Riemann tensor (B.6) then shows that in the final expression of Eq. (B.27),

$$R_{j00k} = \frac{1}{2}\partial_0^2 h_{jk}\,,$$

replacing on the left a time index 0 with z implies replacing on the right-hand side a ∂_0 with $-\partial_z$. Finally, we note that for a planar wave we have $\partial_x h_{\alpha\beta} = \partial_y h_{\alpha\beta} = 0$. With $h_{xx} = -h_{yy} = h_+$ and $h_{xy} = h_{yx} = h_\times$, we then find the TT analog of Eq. (E.88) as

$$\begin{aligned}
&R_{x0x0} = -R_{y0y0} = -R_{xzx0} = R_{yzy0} R_{xzxz} = -R_{yzyz} = -\frac{1}{2}\partial_0^2 h_+\,,\\
&R_{z0x0} = -R_{zTxz} = -R_{yxy0} = R_{yxyz} = 0\,,\\
&R_{z0z0} = -R_{xyxy} = 0\,.
\end{aligned} \tag{E.90}$$

Since $x^0 = T$ and $\partial_u = \partial_T$, this equals Eq. (E.88) if

$$\boxed{h_+ = \frac{2c}{r}\,.} \tag{E.91}$$

In words, the plus polarization strain is equal to the Bondi news function times a distance scaling $2/r$. The cross polarization mode $h_\times$ vanishes here due to axisymmetry. It is recovered in the general, non-axisymmetric case as the imaginary component of a then complex news function. This is the result of Sachs' [4] generalization of the characteristic formalism which we will briefly review next.

E.5 The characteristic formalism for general spacetimes

A few months after the paper of Bondi *et al* was published, Sachs [4] presented the generalization to general asymptotically flat spacetimes. These calculations are naturally more lengthy and we do not have the time (nor need) to go into the details. Purpose of this section is to briefly summarize Sachs' work, highlight the differences from the axisymmetric case and, most importantly, establish the relation to the cross polarization mode $h_\times$ missing in the axisymmetric case.

The construction of characteristic coordinates proceeds in the same manner as above leading again to the retarded time u, areal radius r along the outgoing light rays and angular coordinates θ and ϕ. The line element is then given by

$$\mathrm{d}s^2 = \frac{\tilde{V}e^{2\beta}}{r}\mathrm{d}u^2 - 2e^{2\beta}\mathrm{d}u\mathrm{d}r + r^2 h_{AB}\left(\mathrm{d}x^A\mathrm{d}x^B - \mathrm{d}x^A U^B\mathrm{d}u - \mathrm{d}x^B U^A\mathrm{d}u + U^A U^B\mathrm{d}u^2\right)\,, \tag{E.92}$$

where $A,\ B = 2,\ 3$ are angular indices and

$$h_{AB}\mathrm{d}x^A\mathrm{d}x^B = \frac{e^{2\gamma}+e^{2\delta}}{2}\mathrm{d}\theta^2 + 2\sin\theta\sinh(\gamma-\delta)\mathrm{d}\theta\mathrm{d}\phi + \sin^2\theta\frac{e^{-2\gamma}+e^{-2\delta}}{2}\mathrm{d}\phi^2\,. \tag{E.93}$$

We have used a tilde in $\tilde{V}$ here, since Sachs applies a minus sign in the definition of this function relative to Bondi's definition, $\tilde{V} = -V$; cf. Eq. (2.8) in [4] and Eq. (14) in [3] where we also bear in mind that Bondi *et al* use the metric signature $+---$ in contrast to Sachs' and ours $-+++$. For completeness, we spell out the metric components for coordinates $x^\alpha = (u,\ r,\ \theta,\ \phi)$,

$$\begin{aligned}
g_{uu} &= \frac{\tilde{V}e^{2\beta}}{r} + \frac{e^{2\gamma}+e^{2\delta}}{2}r^2(U^\theta)^2 + r^2\sin^2\theta\,\sinh(\gamma-\delta)U^\theta U^\phi + \frac{e^{-2\gamma}+e^{-2\delta}}{2}r^2\sin^2\theta\,(u^\phi)^2\,,\\
g_{ur} &= -e^\beta\,,\\
g_{u\theta} &= -r^2\sin\theta\,\sinh(\gamma-\delta)U^\phi - \frac{e^{2\gamma}+e^{2\delta}}{2}U^\theta\,,\\
g_{u\phi} &= -r^2\sin\theta\sinh(\gamma-\delta)U^\theta - \sin^2\theta\,\frac{e^{-2\gamma}+e^{-2\delta}}{2}U^\phi\,,\\
g_{rr} &= g_{r\theta} = \;= g_{r\phi} = 0\,,\\
g_{\theta\theta} &= r^2\frac{e^{2\gamma}+e^{2\delta}}{2}\,,
\end{aligned}$$

$$g_{\theta\phi} = r^2 \sin\theta \sinh(\gamma-\delta)\,,$$

$$g_{\phi\phi} = r^2 \frac{e^{-2\gamma}+e^{-2\delta}}{2} \sin^2\theta\,, \tag{E.94}$$

and we see that we recover the axisymmetric metric (E.21) for $\tilde{V} = -V$, $U^\theta = U$, $U^\phi = 0$ and $\gamma = \delta$. But, imagining how the Ricci tensor might look like for this monster of a metric, we also feel vindicated in chickening out on doing the general case in full detail.

The Einstein equations for this metric are most conveniently decomposed into projections with a null tetrad composed of four vectors – two real vectors k and $\boldsymbol{\ell}$ and two complex vectors m and $\overline{\mathsf{m}}$ conjugate to each other[5] – whose inner products are

$$\boldsymbol{g}(\mathsf{k},\boldsymbol{\ell}) = 1\,, \qquad \boldsymbol{g}(\mathsf{m},\overline{\mathsf{m}}) = 1\,, \tag{E.95}$$

$$\boldsymbol{g}(\mathsf{k},\mathsf{k}) = \boldsymbol{g}(\boldsymbol{\ell},\boldsymbol{\ell}) = \boldsymbol{g}(\mathsf{m},\mathsf{m}) = \boldsymbol{g}(\boldsymbol{\ell},\mathsf{m}) = \boldsymbol{g}(\mathsf{k},\mathsf{m}) = \boldsymbol{g}(\overline{\mathsf{m}},\overline{\mathsf{m}}) = \boldsymbol{g}(\boldsymbol{\ell},\overline{\mathsf{m}}) = \boldsymbol{g}(\mathsf{k},\overline{\mathsf{m}}) = 0\,.$$

Since a tensor is uniquely defined in terms of its action on a set of basis vectors, the metric can be expressed in terms of the tetrad as

$$\boldsymbol{g} = \mathsf{k}\otimes\boldsymbol{\ell} + \boldsymbol{\ell}\otimes\mathsf{k} + \mathsf{m}\otimes\overline{\mathsf{m}} + \overline{\mathsf{m}}\otimes\mathsf{m}\,. \tag{E.96}$$

The specific choice of tetrad used in Sachs' calculation is given in terms of the metric variables by Eqs. (A.10)-(A.13) in Ref. [4], but the complicated expressions are not important for our discussion[6]. We note, however, that as $r\to\infty$, they approach their flat-spacetime limits

$$\mathsf{k}^\alpha \simeq \left[-1,\,\tfrac{1}{2},\,0,\,0\right]\,,$$

$$\ell^\alpha \simeq [0,\,1,\,0,\,0]\,,$$

$$\mathsf{m}^\alpha \simeq \left[0,\,0,\,\tfrac{i+\mathrm{i}}{2r},\,\tfrac{1-\mathrm{i}}{2r\sin\theta}\right]\,. \tag{E.97}$$

In terms of the 3+1 unit vectors of Eqs. (E.83)-(E.86), we can write the asymptotic limit of the tetrad vectors as

$$\mathsf{k} \simeq -\boldsymbol{\partial}_u + \frac{1}{2}\boldsymbol{\partial}_r = -\boldsymbol{\partial}_T + \frac{\boldsymbol{\partial}_T+\boldsymbol{\partial}_R}{2} = -\frac{1}{2}(\boldsymbol{\partial}_T - \boldsymbol{\partial}_R) = -\frac{1}{2}(\mathbf{e}_T - \mathbf{e}_R) = -\frac{1}{2}(\mathbf{e}_T - \mathbf{e}_z)\,,$$

$$\boldsymbol{\ell} \simeq \boldsymbol{\partial}_r = \boldsymbol{\partial}_T + \boldsymbol{\partial}_R = \boldsymbol{\partial}_T + \boldsymbol{\partial}_z = \mathbf{e}_T + \mathbf{e}_Z = \mathbf{e}_T + \mathbf{e}_R\,,$$

[5] Unsurprisingly, there is a large variation of the letters used for these null tetrad vectors. The most common alternative is the use of n in place of k, but readers should not be surprised to see any combination of letters imaginable in the literature. Note that both, Bondi *et al* [3] and Sachs [4], use different notations from ours and from each other.

[6] Note that Sachs denotes our ℓ_α by k_α (hence our decision to use different fonts for our tetrad vectors) and has a sign inconsistency between the definition of $k_\alpha = u_{,\alpha} = (x^0)_{,\alpha}$ in Eq. (2.2) and the expression in the second last line of Eq. (A.10) where $k_\alpha = [-1, 0, 0, 0]$. We assume here the + version, but it does not matter much since his k^α (our ℓ^α) will only appear hereafter as a factor in expressions that vanish.

$$\mathbf{m} \simeq \frac{\mathbf{e}_\theta + \mathbf{e}_\phi}{2} + \mathrm{i}\,\frac{\mathbf{e}_\theta - \mathbf{e}_\phi}{2} = \frac{\mathbf{e}_x + \mathbf{e}_y}{2} + \mathrm{i}\,\frac{\mathbf{e}_x - \mathbf{e}_y}{2}\,. \tag{E.98}$$

Projecting the Einstein equations $R_{\alpha\beta} = 0$ onto the tetrad vectors results in a hierarchy of equations analogous to those of Bondi's axisymmetric case in Sec. E.3.

(i) 6 *main equations* which subdivide into

  (a) 4 *hypersurface equations* $R_{\alpha\beta}\ell^\alpha\ell^\beta = R_{\alpha\beta}\ell^\alpha \mathsf{m}^\beta = R_{\alpha\beta}\mathsf{m}^\alpha\overline{\mathsf{m}}^\beta = 0\,,$

  (b) 2 *standard equations*, $R_{\alpha\beta}\mathsf{m}^\alpha\mathsf{m}^\beta = 0\,,$

(ii) 1 *trivial equation* $R_{\alpha\beta}\ell^\alpha\mathsf{k}^\beta = 0\,,$

(iii) 3 *supplementary equations* $R_{\alpha\beta}\mathsf{k}^\alpha\mathsf{m}^\beta = R_{\alpha\beta}\mathsf{k}^\alpha\mathsf{k}^\beta = 0\,.$

As in the Bondi case, one can show the following: (i) The trivial equation is an algebraic consequence of the main equations. (ii) The supplementary equations hold everywhere provided they hold on a hypersurface r = const and the main equations hold everywhere. (iii) the hypersurface equations contain no u derivatives of the metric variables [cf. Eqs. (E.37)-(E.39)] while the standard equations contain time derivatives $\partial_u\gamma$ and $\partial_u\delta$ [cf. Eq. (E.40)].

The construction of a solution to the Einstein equations then consists in the determination of the 6 metric components $\tilde{V}$, U^A, β, γ and δ as functions of the coordinates (u, r, θ, ϕ). This is achieved as follows.

(1) We need to prescribe 2 functions of (r, θ, ϕ) as initial data for the variables γ, δ at u_0 and 2 functions of (u, θ, ϕ) for their time derivatives $\partial_u c$. The complex function c is the Bondi news function generalized to non-axisymmetric spacetimes and represents the leading-order term in the series expansion of γ and δ analogous to Eq. (E.53),

$$\frac{1}{2}[(\delta + \mathrm{i}\gamma)(1 - \mathrm{i})] = cr^{-1} + \mathcal{O}(r^{-2}) \tag{E.99}$$

$$\Rightarrow \quad \partial_u c(u, \theta, \phi) = \frac{1}{2} \lim_{r\to\infty} \left[r(\delta + \mathrm{i}\gamma)(1 - \mathrm{i})\right] . \tag{E.100}$$

We also need to prescribe three functions of (θ, ϕ), a complex-valued N and a real M, as initial data for three constants of integration.

(2) On the initial hypersurface $u = u_0$, the four hypersurface equations result in ordinary differential equations along the null rays whose integration gives us the remaining metric functions β, U^A and $\tilde{V}$. Here we need N and M as functions of integration.

(3) The two standard equations then determine the time evolution of γ and δ which we update to the next time $u_0 + \delta u$. Here we need $\partial_u c$ as two further functions of integration.

(4) The supplementary equations determine the time evolution of the functions of integration, N and M, in terms of the news function c in analogy to Eqs. (E.59), (E.60). Hereafter, we repeat the process starting with step (1) at the updated time value.

As in the case of axisymmetry, the field equations combined with the requirement of asymptotic flatness and no incoming radiation leads to a series expansion of the metric functions now given by Eq. (E.99) and

$$\begin{aligned}
\beta &= -\frac{c\bar{c}}{4} r^{-2} + \mathcal{O}(r^{-3}) , \\
U^\theta + \mathrm{i}U^\phi &= -\left(\partial_\theta c + 2\cot\theta\, c - \frac{\mathrm{i}}{\sin\theta}\partial_\phi c\right) r^{-2} + \mathcal{O}(r^{-3}) , \\
\tilde{V} &= -r + 2M + \mathcal{O}(r^{-1}) .
\end{aligned} \tag{E.101}$$

The relation between the news function c and the gravitational-wave strain is obtained by computing the projections of the Riemann tensor onto the tetrad vectors $\mathbf{k}$, $\boldsymbol{\ell}$, $\mathbf{m}$ and $\overline{\mathbf{m}}$. The resulting series expansion in $1/r$ for the 10 independent components of the Riemann tensor in vacuum is given in Eqs.(5.1)-(5.5) of Ref. [4] in accordance with the peeling theorem which describes the asymptotic behaviour of the Weyl tensor at null infinity [23]. In the limit $r \to \infty$, the Riemann tensor is dominated by two components,[7]

$$R_{\mu\nu\rho\sigma}\mathsf{k}^\mu\mathsf{m}^\nu\mathsf{k}^\rho\mathsf{m}^\sigma = -\frac{\mathrm{i}}{r}\partial_u^2\bar{c} + \mathcal{O}(r^{-2})\,. \tag{E.102}$$

We wish to evaluate these components in the limit $r \to \infty$ where the tetrad vectors are related to the unit vectors along the space-time coordinates by Eq. (E.98), so that

$$\begin{aligned} R_{\mu\nu\rho\sigma}\mathsf{k}^\mu\mathsf{m}^\nu\mathsf{k}^\rho\mathsf{m}^\sigma &\simeq \mathbf{R}(\mathbf{k},\mathbf{m},\mathbf{k},\mathbf{m}) \\ &\simeq \boldsymbol{R}\left(-\frac{\mathbf{e}_T-\mathbf{e}_R}{2},\ \frac{\mathbf{e}_\theta+\mathbf{e}_\phi}{2}+\mathrm{i}\frac{\mathbf{e}_\theta-\mathbf{e}_\phi}{2},\ -\frac{\mathbf{e}_T-\mathbf{e}_R}{2},\ \frac{\mathbf{e}_\theta+\mathbf{e}_\phi}{2}+\mathrm{i}\frac{\mathbf{e}_\theta-\mathbf{e}_\phi}{2}\right) \\ &\simeq \boldsymbol{R}\left(-\frac{\mathbf{e}_T-\mathbf{e}_z}{2},\ \frac{\mathbf{e}_x+\mathbf{e}_y}{2}+\mathrm{i}\frac{\mathbf{e}_x-\mathbf{e}_y}{2},\ -\frac{\mathbf{e}_T-\mathbf{e}_z}{2},\ \frac{\mathbf{e}_x+\mathbf{e}_y}{2}+\mathrm{i}\frac{\mathbf{e}_x-\mathbf{e}_y}{2}\right)\,. \end{aligned} \tag{E.103}$$

In total, this gives us a sum of 64 individual components of the Riemann tensor, but this calculation is greatly simplified if we recall that the Riemann tensor for outgoing radiation satisfies $R_{z\alpha\beta\gamma} = -R_{T\alpha\beta\gamma}$. A lot of terms then cancel or trivially add up and we obtain

$$\lim_{r\to\infty} R_{\mu\nu\rho\sigma}\mathsf{k}^\mu\mathsf{m}^\nu\mathsf{k}^\rho\mathsf{m}^\sigma = R_{TxTy} + \mathrm{i}\frac{R_{TxTx}-R_{TyTy}}{2} \stackrel{!}{=} -\mathrm{i}\frac{\partial_u^2\bar{c}}{r}\,. \tag{E.104}$$

In the linearized regime, Eq. (B.27) gives us

$$\begin{aligned} R_{TxTx} &= -\frac{1}{2}\partial_T^2 h_{xx} = -\frac{1}{2}\partial_T^2 h_+\,, \\ R_{TxTy} &= -\frac{1}{2}\partial_T^2 h_{xy} = -\frac{1}{2}\partial_T^2 h_\times\,, \\ R_{TyTy} &= -\frac{1}{2}\partial_T^2 h_{yy} = +\frac{1}{2}\partial_T^2 h_+\,. \end{aligned} \tag{E.105}$$

Inserting these expressions into Eq. (E.104) yields

$$\boxed{h_+ = \frac{2}{r}\mathsf{Re}(c)\,, \qquad h_\times = \frac{2}{r}\mathsf{Im}(c)\,.} \tag{E.106}$$

This generalizes Eq. (E.91) from the axisymmetric case by adding the cross polarization mode in terms of the imaginary part of the news function.

The time evolution of the Bondi mass

$$m(u) = \frac{1}{4\pi}\int_0^\pi\int_0^{2\pi} M(u,\theta,\phi)\sin\theta\,\mathrm{d}\phi\,\mathrm{d}\theta\,,$$

[7] Note that Sachs uses a different sign convention, swapping the last two indices of the Riemann tensor relative to our convention, which leads to the minus sign on our right-hand side compared to his Eq. (5.1).

is obtained from the r^{-2} terms of the series expansion of the supplementary equations analogous to Eq. (E.59) which give us $\partial_u M$ in terms of c. Integrating over the surface of a sphere gives us the following result.

Proposition: The time evolution of the Bondi mass for non-axisymmetric spacetimes is given by

$$\begin{aligned}\partial_u m &= -\frac{1}{4\pi}\int_0^\pi\int_0^{2\pi}|\partial_u c|^2\sin\theta\,\mathrm{d}\phi\,\mathrm{d}\theta \\ &= -\lim_{r\to\infty}\frac{r^2}{16\pi}\int_0^\pi\int_0^{2\pi}[(\partial_T h_+)^2+(\partial_T h_\times)^2]\sin\theta\,\mathrm{d}\phi\,\mathrm{d}\theta\,.\end{aligned} \tag{E.107}$$

Note that the right-hand side is manifestly non-positive, so m remains constant or decreases. For stationary spacetimes, the mass is constant.

We can interpret this result in physical terms by considering a source that passes from a time independent state with mass $m_{\rm ini}$ through a dynamical phase before settling down into another time independent state with mass $m_{\rm fin}$. The amount of GW energy radiated to infinity during the dynamical phase is then given by $m_{\rm ini} - m_{\rm fin}$.

Even though we have discussed the characteristic formulation for asymptotically flat spacetimes, it can and has been employed with great success also for spacetimes with different asymptotic behaviour, such as anti-de Sitter. The reason for our focus on asymptotic flatness lies in the identification of the news function with the GW strain of linearized theory which holds in this form only in asymptotic flatness. The identification of gravitational radiation in fully non-linear GR was, of course, our initial motivation for studying the characteristic formalism in the first place, even though we may have temporarily forgotten about this... The key limitation of characteristic simulations is the breakdown of the coordinate system once null rays cross – which generically happens in BH binary spacetimes. The numerical community still investigates possible improvements of characteristic methods to simulate compact binaries, but as of now, all numerical relativity simulations of compact binaries have used so-called 3+1 methods. How this is done, is the next chapter in our voyage.

F The ADM 3+1 formulation

In our classification of PDEs in Sec. C, we have distinguished hyperbolic, parabolic and elliptic differential equations based on the existence or absence of characteristic surfaces, i.e. surfaces where the specification of initial data is not sufficient to determine a solution in a neighbourhood of the surface. We have also seen that information propagates along curves that make up the characteristic surfaces; see for example our discussion of the wave equation in characteristic coordinates on page 26. It is therefore common to view hyperbolic and parabolic PDEs – both of which admit characteristic surfaces – as *time evolution* or *initial value problems* whereas elliptic PDEs are *boundary value problems*. The idea is that time evolution problems require the specification of initial data whose evolution in time is determined by the system of PDEs. For example, if we prescribe the temperature profile along a metal bar, the heat equation will determine how the temperature at every point will change in time. A more complex example working in the same way is the weather forecast which computes the time evolution of the present weather conditions according to the equations of hydrodynamics in the presence of a gravitational field. Boundary value problems, in contrast, describe stationary configurations constrained by specified boundary conditions. For example, we can compute the shape of a drum head whose surface is subjected to the pull of gravity while being fixed to the drum's frame with a specified tension. This distinction of time evolution and boundary value problems is also motivated by the development of numerical tools employed to solve them; elliptic solvers operate differently from time stepping algorithms.

We have already gained some insight into the structure of the Einstein equations in Sec. D, where we have seen that the vacuum equations $R_{\alpha\beta} = 0$ determine the evolution of some, but not all, components of the spacetime metric. In this section, we will analyze this feature of the Einstein equations in more detail and also introduce the canonical formulation of the equations as a constrained evolution problem.

F.1 Spacetime foliations, induced metric and extrinsic curvature

The canonical 3+1 split of the Einstein equations dates back to the work of Arnowitt, Deser and Misner [5] and is commonly referred to as the ADM formulation. Most practical work in numerical relativity, however, is based on York's [6] reformulation which expresses the time derivative of the metric in terms of the extrinsic curvature rather than the canonical momentum variables. In spite of this difference, York's equations are still commonly called the ADM equations and we shall follow this convention. Our derivation will be self-contained but readers interested in more details can find these in Gourgoulhon's review [24].

Let us start by considering a manifold $\mathcal{M}$ equipped with a metric $\boldsymbol{g}$ and a hypersurface Σ given in the form of a level surface $t(x^\alpha) = \text{const}$. Eventually, t will become our time coordinate, and we consider globally hyperbolic spacetimes as defined on page 40; for the moment, however, we allow $\mathbf{d}t$ to be either timelike or spacelike and we even allow $\boldsymbol{g}$ to be either a Lorentzian (signature +2) or Riemannian (signature +4) metric. Many of our definitions and derivations hold for either case and find practical applications; alternatively to hypersurfaces of constant time, we may, for example, deal with surfaces of constant radius.

<u>Def. :</u> Let $\mathcal{M}$ be a manifold with Lorentzian or Riemannian metric $\boldsymbol{g}$ and Σ a hypersurface defined as a level set $t(x^\alpha) = \text{const}$. We define the *unit normal* of this hypersurface as

$$\boldsymbol{n} := \mp\alpha\mathbf{d}t\,, \qquad \text{where} \qquad \alpha = \sqrt{\mp||\mathbf{d}t||^2}^{\,-1}\,, \tag{F.1}$$

so that $||\boldsymbol{n}||^2 = n^\mu n_\mu = \mp 1$. Here, and in the following, the upper sign is used if $\mathbf{d}t$ is timelike and the lower sign if $\mathbf{d}t$ is spacelike. Note that we have two minus signs for timelike $\mathbf{d}t$; the first implies that $\boldsymbol{n}$ is future pointing, $\langle\mathbf{d}t, \boldsymbol{n}\rangle = -\alpha||\mathbf{d}t||^2 > 0$, and the second ensures a positive argument inside the square root. The function α is called the *lapse function* or *lapse* for short. We furthermore define the *projector*

$$\perp^\alpha{}_\beta := \delta^\alpha{}_\beta \pm n^\alpha n_\beta\,, \tag{F.2}$$

and the *acceleration vector* or *acceleration* for short,

$$a_\beta := n^\mu \nabla_\mu n_\beta \qquad \Leftrightarrow \qquad \boldsymbol{a} := \nabla_{\boldsymbol{n}}\boldsymbol{n}\,. \tag{F.3}$$

<u>Def. :</u> A vector $\boldsymbol{X}$ is *tangent to* Σ if $\langle\mathbf{d}t, \boldsymbol{X}\rangle = 0$ or, equivalently, $\boldsymbol{n}\cdot\boldsymbol{X} = 0$. The *projection of a tensor* $\boldsymbol{T}$ of arbitrary rank is

$$\perp T^{\alpha\beta\ldots}{}_{\gamma\delta\ldots} := \perp^\alpha{}_\mu \perp^\beta{}_\nu \ldots \perp^\rho{}_\gamma \perp^\sigma{}_\delta \ldots T^{\mu\nu\ldots}{}_{\rho\sigma\ldots}\,, \tag{F.4}$$

i.e. we apply one projector for each index of $\boldsymbol{T}$.

These definitions imply the following.

(1) $\perp^\alpha{}_\mu n^\mu = n^\alpha \pm n^\alpha(n_\mu n^\mu) = 0$, since $n^\mu n_\mu = \mp 1$.

(2) The acceleration is tangent to Σ: $n^\mu a_\mu = n^\mu n^\rho \nabla_\rho n_\mu = \frac{1}{2} n^\rho \nabla_\rho (n^\mu n_\mu) = 0$.

(3) $\perp^\alpha{}_\mu \perp^\mu{}_\beta = (\delta^\alpha{}_\mu \pm n^\alpha n_\mu)(\delta^\mu{}_\beta \pm n^\mu n_\beta) = \delta^\alpha{}_\beta \pm 2n^\alpha n_\beta + \underbrace{(n_\mu n^\mu)}_{=\mp 1} n^\alpha n_\beta = \perp^\alpha{}_\beta\,,$

i.e. $\perp^\alpha{}_\beta$ is idempotent which is the defining property of a projector.

(4) For any vector $\boldsymbol{V}$, $\perp\boldsymbol{V}$ is tangent to Σ: $\quad \perp^\alpha{}_\mu V^\mu n_\alpha = V^\alpha n_\alpha \pm \underbrace{(n^\alpha n_\alpha)}_{=\mp 1} n_\mu V^\mu = 0.$

If $\boldsymbol{V}$ is already tangent to Σ, then $\perp^\alpha{}_\mu V^\mu = (\delta^\alpha{}_\mu + n^\alpha n_\mu)V^\mu = V^\alpha$.

(5) For any vectors $\boldsymbol{V}$, $\boldsymbol{W}$ tangent to Σ, we have $g_{\alpha\beta}V^\alpha W^\beta = \perp_{\alpha\beta} V^\alpha W^\beta$.

The last two properties apply in analogy to one-forms and to each component of a tensor of higher rank. This motivates the following definition.

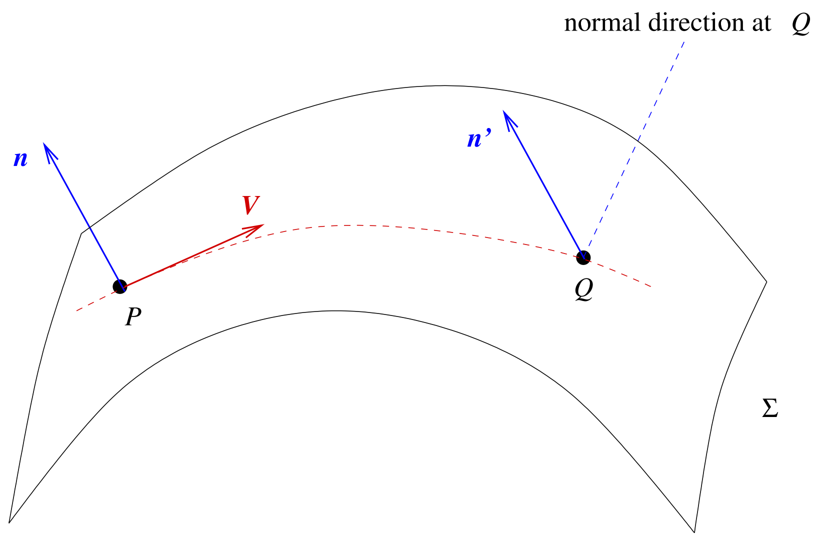


Figure 12: We take the unit normal $\boldsymbol{n}$ at point P of a hypersurface Σ and parallel transport it along the integral curve of the vector field $\boldsymbol{V}$ to the point Q. The resulting vector $\boldsymbol{n}'$ will in general not be normal to Σ at Q. Its deviation from the normal direction is a measure for the curved embedding of Σ inside the spacetime $\mathcal{M}$ and defines the extrinsic curvature.

Def. : The *induced metric* on Σ is

$$\gamma_{\alpha\beta} = \perp_{\alpha\beta} = g_{\alpha\beta} \pm n_\alpha n_\beta\,. \tag{F.5}$$

It is sometimes also called the *first fundamental form*. Note that we have two symbols for the same object here, $\gamma_{\alpha\beta} = \perp_{\alpha\beta}$. We will use both in the following, depending on whether the emphasis is on its character as a projector or a metric.

Let us now consider a vector field $\boldsymbol{V}$ that is tangent to Σ at every point and parallel transport the unit normal vector $\boldsymbol{n}$ from point P to Q along $\boldsymbol{V}$ as illustrated in Fig. 12. Recall that the equation for parallel transport along the integral curve of a vector field is given by

$$\nabla_{\boldsymbol{V}}\boldsymbol{n} = 0 \qquad \Leftrightarrow \qquad V^\mu \nabla_\mu n^\alpha = 0\,. \tag{F.6}$$

We now ask the question whether $\boldsymbol{n}$ remains normal to Σ as we parallel transport it from P to Q. In other words, does the inner product of $\boldsymbol{n}$ with an arbitrary vector field $\boldsymbol{Y}$ tangent to Σ remain zero under parallel transport? The answer is that in general it does not, since

$$V^\mu \nabla_\mu (Y^\alpha n_\alpha) = Y^\alpha \underbrace{V^\mu \nabla_\mu n_\alpha}_{=0} + n_\alpha V^\mu \nabla_\mu Y^\alpha\,, \tag{F.7}$$

does not vanish. As illustrated in Fig. 12, this departure from orthogonality of $\boldsymbol{n}$ under parallel transport is a consequence of the curved embedding of Σ in $\mathcal{M}$ which we now phrase in concrete mathematical terms.

Def. : For any extension of the vector field $\boldsymbol{n}$ in a neighbourhood of Σ such that $n^\mu n_\mu = \mp 1$, the *extrinsic curvature* or *second fundamental form* is defined as the map

$$\boldsymbol{K} : (\boldsymbol{V}, \boldsymbol{W}) \mapsto \boldsymbol{n}\Big(\nabla_{\perp \boldsymbol{V}}(\perp \boldsymbol{W})\Big) \qquad \Leftrightarrow \qquad K_{\mu\nu}V^\mu W^\nu := n_\nu \perp V^\mu \nabla_\mu(\perp W^\nu)\,. \tag{F.8}$$

Note that we do not require the vector fields $\boldsymbol{V}$ and $\boldsymbol{W}$ to be tangent to Σ in this definition.

Proposition: Independent of the extension, the extrinsic curvature tensor is given by

$$K_{\alpha\beta} = -\perp^\mu{}_\alpha \nabla_\mu n_\beta = -\nabla_\alpha n_\beta \mp n_\alpha a_\beta\,. \tag{F.9}$$

Proof. For two vector fields $\boldsymbol{V}$, $\boldsymbol{W}$ we find,

$$K_{\mu\nu}V^\mu W^\nu = n_\nu \perp V^\mu \nabla_\mu(\perp W^\nu) = -\perp V^\mu \perp W^\nu \nabla_\mu n_\nu = -\perp^\mu{}_\alpha V^\alpha \perp^\nu{}_\beta W^\beta \nabla_\mu n_\nu\,.$$

This relation holds for arbitrary $\boldsymbol{V}$, $\boldsymbol{W}$, so that the components of $\boldsymbol{K}$ are

$$K_{\alpha\beta} = -\perp^\mu{}_\alpha \perp^\nu{}_\beta \nabla_\mu n_\nu\,. \tag{F.10}$$

Now let n'_α be another extension in the neighbourhood of Σ and define $m_\alpha := n'_\alpha - n_\alpha$. Then at every point on Σ we have $m_\alpha = 0$ and

$$\begin{aligned} V^\alpha W^\beta(K_{\alpha\beta} - K'_{\alpha\beta}) &= \perp^\mu{}_\alpha \perp^\nu{}_\beta V^\alpha W^\beta \nabla_\mu m_\nu = \perp V^\mu\Big[\perp W^\nu \nabla_\mu m_\nu + \underbrace{m_\nu}_{=0} \nabla_\mu(\perp W^\nu)\Big] \\ &= \perp V^\mu \nabla_\mu(m_\nu \perp W^\nu) = 0\,, \end{aligned}$$

because the last derivative is taken along a direction tangent to Σ where the argument $m_\nu \perp W^\nu$ vanishes.

Finally, we can eliminate one of the projection operators in Eq. (F.10) since

$$n^\mu \nabla_\alpha n_\mu = \frac{1}{2}\nabla_\alpha(n_\mu n^\mu) = 0$$

$$\Rightarrow \quad K_{\alpha\beta} = -\perp^\mu{}_\alpha \perp^\nu{}_\beta \nabla_\mu n_\nu = -\perp^\mu{}_\alpha(\delta^\nu{}_\beta \pm n^\nu n_\beta)\nabla_\mu n_\nu = -\perp^\mu{}_\alpha \nabla_\mu n_\beta\,. \tag{F.11}$$

This also gives us

$$K_{\alpha\beta} = -\nabla_\alpha n_\beta \mp n_\alpha \underbrace{n^\mu \nabla_\mu n_\beta}_{=a_\beta}\,. \tag{F.12}$$

□

Proposition: The extrinsic curvature is symmetric,

$$K_{\alpha\beta} = K_{\beta\alpha}, \tag{F.13}$$

and tangent to Σ in both indices,

$$K_{\alpha\beta}n^{\alpha} = 0 = K_{\alpha\beta}n^{\beta}. \tag{F.14}$$

The trace of the extrinsic curvature is

$$K := g^{\mu\nu}K_{\mu\nu} = \gamma^{\mu\nu}K_{\mu\nu}. \tag{F.15}$$

Proof. Recalling Eq. (F.1), we can write

$$\nabla_\mu n_\nu = \mp\nabla_\mu(\alpha \mathbf{d}t_\nu) = \mp\alpha\nabla_\mu\nabla_\nu t + (\nabla_\mu\alpha)\frac{n_\nu}{\alpha}$$
$$\Rightarrow \quad K_{\alpha\beta} = -\perp^{\mu}{}_{\alpha}\perp^{\nu}{}_{\beta}\nabla_\mu n_\nu = \pm\alpha\perp^{\mu}{}_{\alpha}\perp^{\nu}{}_{\beta}\nabla_\mu\nabla_\nu t + 0\,. \tag{F.16}$$

In general relativity we use the Levi-Civita connection which is torsion free, so that $\nabla_\mu\nabla_\nu t = \nabla_\nu\nabla_\mu t$ for any scalar field t. The tangent nature follows directly from Eq. (F.10). This also implies

$$K = g^{\mu\nu}K_{\mu\nu} = \gamma^{\mu\nu}K_{\mu\nu} \mp \underbrace{n^\mu n^\nu K_{\mu\nu}}_{=0}\,. \tag{F.17}$$

□

From now on, we shed the burden of multiple signs and restrict our discussion to the case of Lorentzian metrics and spacelike hypersurfaces Σ, i.e. the case of timelike normals $\mathbf{d}t$ and $\boldsymbol{n}$. This corresponds to using the upper signs in all expressions of this subsection, i.e. henceforth, we use

$$\boldsymbol{n} = -\alpha\mathbf{d}t\,, \qquad n_\mu n^\mu = -1\,, \qquad \perp^{\alpha}{}_{\beta} = \delta^{\alpha}{}_{\beta} + n^\alpha n_\beta\,, \qquad \gamma_{\alpha\beta} = g_{\alpha\beta} + n_\alpha n_\beta\,. \tag{F.18}$$

By considering both cases so far, we merely wanted to emphasize that the formalism can be applied to both space- or timelike hypersurfaces with simply some changes in signs. The main application in our notes, however, is the derivation of time evolution equations where the slices Σ are spatial.

F.2 Intrinsic curvature

The extrinsic curvature describes the embedding of the hypersurface Σ inside the four-dimensional spacetime manifold $\mathcal{M}$. The hypersurface may, however, also have intrinsic curvature in the sense of a non-vanishing Riemann tensor and its manifestation through geodesic deviation and a change of vectors under parallel transport along closed curves. The intrinsic curvature is a purely three-dimensional phenomenon and thus concerns exclusively tensors that are tangent to Σ in all components, as for example a rank $\binom{0}{2}$ tensor $T_{\alpha\beta}$ with $T_{\alpha\mu}n^\mu = 0 = T_{\mu\beta}n^\mu$. The Riemann tensor associated with the three-dimensional hypersurface is different from its four-dimensional counterpart and is denoted in the following by $\mathcal{R}_{\alpha\beta\gamma\delta}$. Eventually, we will see that the spacetime Riemann tensor can be regarded as a combination of its three-dimensional counterpart and the extrinsic curvature $K_{\alpha\beta}$. As a first step in our derivation of the corresponding relations, we define the three-dimensional covariant derivative.

Def. : Let $T^{\alpha\ldots}{}_{\beta\ldots}$ be a tensor of rank $\binom{r}{s}$ tangent to Σ in all components, i.e. $T^{\alpha\ldots}{}_{\beta\ldots}n_\alpha = T^{\alpha\ldots}{}_{\beta\ldots}n^\beta = \ldots = 0$. The *three-dimensional* or *spatial* covariant derivative of $\boldsymbol{T}$ is the rank $\binom{r}{s+1}$ tensor

$$D_\mu T^{\alpha\ldots}{}_{\beta\ldots} := \perp^\rho{}_\mu \perp^\alpha{}_\sigma \perp^\tau{}_\beta \ldots \nabla_\rho T^{\sigma\ldots}{}_{\tau\ldots}\,. \tag{F.19}$$

In words, we take the four-dimensional covariant derivative and project on every free index.

Proposition: This definition implies that for any vector field $\boldsymbol{X}$ tangent to Σ,

$$(D_{\boldsymbol{X}}\boldsymbol{T}) = \perp(\nabla_{\boldsymbol{X}}\boldsymbol{T}) \quad \text{or} \quad X^\mu D_\mu T^{\alpha\ldots}{}_{\beta\ldots} = \perp^\alpha{}_\sigma \perp^\tau{}_\beta \ldots (X^\rho \nabla_\rho T^{\sigma\ldots}{}_{\tau\ldots})\,.$$

Proof. Since $\perp^\rho{}_\mu X^\mu = X^\rho$, we find

$$\begin{aligned}(D_{\boldsymbol{X}}\boldsymbol{T})^{\alpha\ldots}{}_{\beta\ldots} &= X^\mu D_\mu T^{\alpha\ldots}{}_{\beta\ldots} = X^\mu \perp^\rho{}_\mu \perp^\alpha{}_\sigma \perp^\tau{}_\beta \ldots \nabla_\rho T^{\sigma\ldots}{}_{\tau\ldots} \\ &= \perp^\alpha{}_\sigma \perp^\tau{}_\beta \ldots (X^\rho \nabla_\rho T^{\sigma\ldots}{}_{\tau\ldots}) = \perp(\nabla_{\boldsymbol{X}}\boldsymbol{T})^{\alpha\ldots}{}_{\beta\ldots}\,.\end{aligned} \tag{F.20}$$

□

Proposition: The derivative defined by Eq. (F.19) is a covariant derivative for tensors tangent to Σ. It is torsion free and compatible with the spatial metric $\gamma_{\alpha\beta}$. By the fundamental theorem of Riemannian geometry, the connection associated with this covariant derivative is unique.

Proof. The covariant derivative is defined as a map from two smooth vector field $\boldsymbol{X}$, $\boldsymbol{V}$ to a smooth vector field $\nabla_{\boldsymbol{X}}\boldsymbol{V}$ such that the mapping is linear in the first argument, linear with regard to addition in the second argument and obeys Leibniz rule for scalar multiplication of the second argument. Furthermore, the covariant derivative applied to a scalar reduces to the partial derivative. We first show that the derivative defined in Eq. (F.19) satisfies these requirements and thus constitutes a covariant derivative. Consider for this purpose three smooth vector fields $\boldsymbol{X}$, $\boldsymbol{Y}$ and $\boldsymbol{V}$ tangent to Σ and let f, g be scalar functions on Σ. We find,

(1) Covariant derivative of a scalar:

$$(D_{\boldsymbol{X}} f) = X^\mu D_\mu f = X^\mu \perp^\rho{}_\mu \nabla_\rho f = X^\mu \perp^\rho{}_\mu \partial_\rho f = X^\rho \partial_\rho f\,, \tag{F.21}$$

since $\boldsymbol{X}$ is tangent to Σ and, therefore, $\perp^\mu{}_\rho X^\rho = X^\mu$. This applies to any spatial vector $\boldsymbol{X}$, so that we can write $D_\mu f = \partial_\mu f$ as required for the covariant derivative of a scalar.

(2) Linearity in the first argument is inherited from the four-dimensional covariant derivative,

$$\begin{aligned} D_{f\boldsymbol{X}+g\boldsymbol{Y}}\boldsymbol{V} &= \perp(\nabla_{f\boldsymbol{X}+g\boldsymbol{Y}}\boldsymbol{V}) = \perp(f\nabla_{\boldsymbol{X}}\boldsymbol{V} + g\nabla_{\boldsymbol{Y}}\boldsymbol{V}) = f\perp\nabla_{\boldsymbol{X}}\boldsymbol{V} + g\perp\nabla_{\boldsymbol{Y}}\boldsymbol{V} \\ &= fD_{\boldsymbol{X}}\boldsymbol{V} + gD_{\boldsymbol{Y}}\boldsymbol{V}\,. \end{aligned}$$

(3) Linearity for addition in the second argument:

$$D_{\boldsymbol{X}}\boldsymbol{V}+D_{\boldsymbol{X}}\boldsymbol{W} = \perp\nabla_{\boldsymbol{X}}\boldsymbol{V}+\perp\nabla_{\boldsymbol{X}}\boldsymbol{W} = \perp[\nabla_{\boldsymbol{X}}\boldsymbol{V}+\nabla_{\boldsymbol{X}}\boldsymbol{W}] = \perp\nabla_{\boldsymbol{X}}(\boldsymbol{V}+\boldsymbol{W}) = D_{\boldsymbol{X}}(\boldsymbol{V}+\boldsymbol{W})\,,$$

since ∇ is linear with respect to addition of the second argument.

(4) Leibniz rule:

$$\begin{aligned} D_{\boldsymbol{X}}(f\boldsymbol{V}) &= \perp\nabla_{\boldsymbol{X}}(f\boldsymbol{V}) = \perp[f\nabla_{\boldsymbol{X}}\boldsymbol{V} + (\nabla_{\boldsymbol{X}}f)\boldsymbol{V}] = f\perp\nabla_{\boldsymbol{X}}\boldsymbol{V} + \perp\boldsymbol{V}\perp(\nabla_{\boldsymbol{X}}f) \\ &= fD_{\boldsymbol{X}}\boldsymbol{V} + \boldsymbol{V}D_{\boldsymbol{X}}f\,, \end{aligned}$$

since ∇ obeys Leibniz rule and $\perp\boldsymbol{V} = \boldsymbol{V}$.

So D_μ as defined in Eq. (F.19) satisfies the requirements for a covariant derivative for scalar and vector fields tangent to Σ. Its operation on general tensors tangent to Σ is obtained by using Leibniz rule. For a one-form $\boldsymbol{\eta}$ tangent to Σ, for example, we obtain

$$(D_{\boldsymbol{X}}\boldsymbol{\eta})(\boldsymbol{Y}) \coloneqq D_{\boldsymbol{X}}\big(\boldsymbol{\eta}(\boldsymbol{Y})\big) - \eta(D_{\boldsymbol{X}}\boldsymbol{Y})\,, \tag{F.22}$$

which holds for any vector $\boldsymbol{Y}$ tangent to Σ and thus fully determines the covariant derivative of $\boldsymbol{\eta}$. Likewise we can define $D_{\boldsymbol{X}}\boldsymbol{T}$ for any tensor $\boldsymbol{T}$ of higher rank.

The second main part of the proof is to show that D_μ is compatible with the induced metric $\gamma_{\alpha\beta}$. We obtain

$$D_\mu\gamma_{\alpha\beta} = \perp^\rho{}_\mu\perp^\sigma{}_\alpha\perp^\tau{}_\beta\nabla_\rho(g_{\sigma\tau} + n_\sigma n_\tau) = 0\,, \tag{F.23}$$

because $\perp^\sigma{}_\alpha n_\sigma = \perp^\tau{}_\beta n_\tau = 0$ and $\nabla_\rho g_{\sigma\tau} = 0$.

Finally, let $\boldsymbol{X}$ and $\boldsymbol{Y}$ be two vector fields tangent to Σ. Then the torsion tensor is defined as the map

$$\begin{aligned} &\boldsymbol{T} : (\boldsymbol{X},\boldsymbol{Y}) \mapsto \boldsymbol{T}(\boldsymbol{X},\boldsymbol{Y}) = D_{\boldsymbol{X}}\boldsymbol{Y} - D_{\boldsymbol{Y}}\boldsymbol{X} - [\boldsymbol{X},\boldsymbol{Y}] \\ \text{or}\quad &T_{\mu\nu}{}^\alpha X^\mu Y^\nu = X^\mu D_\mu Y^\alpha - Y^\mu D_\mu X^\alpha - [\boldsymbol{X},\boldsymbol{Y}]^\alpha\,, \end{aligned} \tag{F.24}$$

where $[\boldsymbol{X},\boldsymbol{Y}]$ is the commutator of $\boldsymbol{X}$ and $\boldsymbol{Y}$. Since the four-dimensional covariant derivative ∇ is torsion free, we find

$$T_{\mu\nu}{}^\alpha X^\mu Y^\nu = X^\mu\perp\nabla_\mu Y^\alpha - Y^\mu\perp\nabla_\mu X^\alpha - [\boldsymbol{X},\boldsymbol{Y}]^\alpha = \perp(X^\mu\nabla_\mu Y^\alpha) - \perp(Y^\mu\nabla_\mu X^\alpha) - [\boldsymbol{X},\boldsymbol{Y}]^\alpha$$

$$
\begin{aligned}
&= \perp^{\alpha}{}_{\rho} X^{\mu}\nabla_{\mu} Y^{\rho} - \perp^{\alpha}{}_{\rho} Y^{\mu}\nabla_{\mu} X^{\rho} - [\boldsymbol{X},\boldsymbol{Y}]^{\alpha} \\
&= X^{\mu}\nabla_{\mu} Y^{\alpha} - Y^{\mu}\nabla_{\mu} X^{\alpha} + n^{\alpha} n_{\rho} X^{\mu}\nabla_{\mu} Y^{\rho} - n^{\alpha} n_{\rho} Y^{\mu}\nabla_{\mu} X^{\rho} - [\boldsymbol{X},\boldsymbol{Y}]^{\alpha} \\
&= n^{\alpha} n_{\rho}\Big(X^{\mu}\nabla_{\mu} Y^{\rho} - Y^{\mu}\nabla_{\mu} X^{\rho}\Big) \;=\; -\,n^{\alpha} Y^{\rho} X^{\mu}\nabla_{\mu} n_{\rho} + n^{\alpha} X^{\rho} Y^{\mu}\nabla_{\mu} n_{\rho} \\
&\overset{(F.9)}{=} n^{\alpha}(X^{\rho}Y^{\mu} - Y^{\rho}X^{\mu})(-K_{\mu\rho} - n_{\mu} a_{\rho}) = 0\,,
\end{aligned}
\tag{F.25}
$$

since $Y^{\mu}n_{\mu} = X^{\mu}n_{\mu} = 0$ and $K_{\mu\rho}$ is symmetric. This holds for arbitrary vector fields $\boldsymbol{X}$, $\boldsymbol{Y}$ tangent to Σ, so the three-dimensional torsion tensor vanishes and D_{α} is torsion free.

□

In a coordinate basis, the connection coefficients $\Gamma^{\alpha}_{\beta\gamma}$ are given in terms of the metric by Eq. (A.1). Likewise, we will see further below how we can express the three-dimensional connection coefficients, which we denote by[8] $\mathsf{\Gamma}^{\alpha}_{\beta\gamma}$, in terms of the Christoffel symbols of the spatial metric $\gamma_{\alpha\beta}$. This, however, requires us to specify a coordinate system adapted to the space-time split. Readers will have noticed that we have in this section formulated relations between three-dimensional objects, i.e. tensors tangent to Σ, in terms of four-dimensional indices α, β, ... This is perfectly fine and straightforward for tensorial quantities, but becomes problematic once we consider non-tensorial expressions like partial derivatives or the Christoffel symbols. The three-dimensional covariant derivative of a vector field, for example, can be written as

$$
D_{\alpha} V^{\beta} = \perp^{\mu}{}_{\alpha} \perp^{\beta}{}_{\nu} \nabla_{\mu} V^{\nu} = \ldots = \perp^{\mu}{}_{\alpha}\Big[\partial_{\mu} V^{\beta} + n^{\beta} n_{\rho}\partial_{\mu} V^{\rho} + \mathsf{\Gamma}^{\beta}_{\rho\mu} V^{\rho}\Big]\,,
\tag{F.26}
$$

where

$$
\mathsf{\Gamma}^{\beta}_{\rho\mu} = \frac{1}{2}\gamma^{\nu\sigma}(\partial_{\rho}\gamma_{\mu\sigma} + \partial_{\mu}\gamma_{\sigma\rho} - \partial_{\sigma}\gamma_{\rho\mu})\,.
\tag{F.27}
$$

While the latter equation has the form we would expect for the Christoffel symbols, the extra terms in Eq. (F.26) indicate that the interpretation of the covariant derivative as the sum of a partial derivative plus connection terms is not clear in this notation. We should not be surprised about this deficiency; we have not provided enough information about how our coordinates take into account the projection from four to three dimensions. We will fill this gap further below and then also find perfectly satisfactory expressions for the three dimensional Christoffel symbols and how they give us the components of the three-dimensional Riemann tensor.

The spatial covariant derivative defined in the previous subsection defines the spatial Riemann tensor $\mathcal{R}_{\alpha\beta\gamma\delta}$ in complete analogy to the four-dimensional Riemann tensor $R_{\alpha\beta\gamma\delta}$.

[8]Note the different symbols, $\mathsf{\Gamma}$ and Γ, for the three- and four-dimensional Christoffel symbols, respectively. While their difference in appearance is not particularly striking, the intended version will usually be clear from the context and, a bit further below, also from the indices (Latin versus Greek).

Def. : Let $\boldsymbol{X}$, $\boldsymbol{Y}$, $\boldsymbol{V}$ be vector fields tangent to the three-dimensional hypersurface Σ with induced metric $\gamma_{\alpha\beta}$. The *three-dimensional Riemann tensor* is defined such that

$$\boldsymbol{\mathcal{R}}(\boldsymbol{X},\boldsymbol{Y})\boldsymbol{V} = D_{\boldsymbol{X}}D_{\boldsymbol{Y}}\boldsymbol{V} - D_{\boldsymbol{Y}}D_{\boldsymbol{X}}\boldsymbol{V} - D_{[\boldsymbol{X},\boldsymbol{Y}]}\boldsymbol{V} \qquad \text{with}$$

$$\Big(\boldsymbol{\mathcal{R}}(\boldsymbol{X},\boldsymbol{Y})\boldsymbol{V}\Big)^{\alpha} = \mathcal{R}^{\alpha}{}_{\beta\gamma\delta}V^{\beta}X^{\gamma}Y^{\delta}\,. \tag{F.28}$$

The *three-dimensional Ricci tensor* and *Ricci scalar* are defined as

$$\mathcal{R}_{\alpha\beta} := \mathcal{R}^{\mu}{}_{\alpha\mu\beta}\,, \qquad \mathcal{R} := \gamma^{\mu\nu}\mathcal{R}_{\mu\nu}\,. \tag{F.29}$$

From this definition we obtain the same symmetry properties as for the four-dimensional Riemann tensor,

$$\mathcal{R}_{\alpha\beta\gamma\delta} = -\mathcal{R}_{\alpha\beta\delta\gamma}\,, \qquad \mathcal{R}_{\alpha\beta\gamma\delta} = \mathcal{R}_{\gamma\delta\alpha\beta}\,, \qquad \mathcal{R}_{\alpha[\beta\gamma\delta]} = 0\,. \tag{F.30}$$

Likewise, the definition (F.28) directly gives us the three-dimensional Ricci identity.

Proposition: A vector field tangent to Σ obeys the three-dimensional Ricci identity

$$(D_{\gamma}D_{\delta} - D_{\delta}D_{\gamma})V^{\alpha} = \mathcal{R}^{\alpha}{}_{\mu\gamma\delta}V^{\mu}\,. \tag{F.31}$$

F.3 The Gauss, Codazzi and Ricci equations

With the three-dimensional Riemann tensor in place, we can now start our derivation of the 3+1 split of the Einstein equations. The first step is to compute all possible time and space projections of the four-dimensional Riemann tensor and express them in terms of the three-dimensional Riemann tensor and the extrinsic curvature. We start with the fully spatial projection of $R^{\alpha}{}_{\beta\gamma\delta}$.

Proposition: The Riemann tensors satisfy the Gauss equation

$$\perp R^{\alpha}{}_{\beta\gamma\delta} = \mathcal{R}^{\alpha}{}_{\beta\gamma\delta} + K^{\alpha}{}_{\gamma}K_{\delta\beta} - K^{\alpha}{}_{\delta}K_{\gamma\beta}\,. \tag{F.32}$$

This implies the contracted and scalar Gauss equations,

$$\begin{aligned}\perp^{\mu}{}_{\alpha}\perp^{\nu}{}_{\beta}R_{\mu\nu} + \perp^{\mu}{}_{\alpha}\perp^{\rho}{}_{\beta}n^{\nu}n^{\sigma}R_{\mu\nu\rho\sigma} &= \mathcal{R}_{\alpha\beta} + KK_{\alpha\beta} - K_{\alpha\mu}K^{\mu}{}_{\beta}\,,\\ R + 2n^{\mu}n^{\nu}R_{\mu\nu} &= \mathcal{R} + K^2 - K^{\mu\nu}K_{\mu\nu}\,.\end{aligned} \tag{F.33}$$

Proof. The Riemann tensor is fully determined by its action on vector fields according to the Ricci identity (F.31). For a vector field $\boldsymbol{V}$ tangent to Σ we find

$$D_{\alpha}D_{\beta}V^{\gamma} = \perp^{\mu}{}_{\alpha}\perp^{\nu}{}_{\beta}\perp^{\gamma}{}_{\rho}\nabla_{\mu}(D_{\nu}V^{\rho}) = \perp^{\mu}{}_{\alpha}\perp^{\nu}{}_{\beta}\perp^{\gamma}{}_{\rho}\nabla_{\mu}\Big(\perp^{\sigma}{}_{\nu}\perp^{\rho}{}_{\lambda}\nabla_{\sigma}V^{\lambda}\Big)\,. \tag{F.34}$$

For the derivative of the projector we find

$$\nabla_\mu \perp^\sigma{}_\nu = \nabla_\mu(\delta^\sigma{}_\nu + n^\sigma n_\nu) = n_\nu \nabla_\mu n^\sigma + n^\sigma \nabla_\mu n_\nu \,. \tag{F.35}$$

Recalling the extrinsic curvature $K_{\alpha\beta} = -\perp^\mu{}_\alpha \nabla_\mu n_\beta = -\perp^\mu{}_\alpha \perp^\nu{}_\beta \nabla_\mu n_\nu$ and using idempotence of the projector, $\perp^\alpha{}_\mu \perp^\mu{}_\beta = \perp^\alpha{}_\beta$, we obtain

$$\begin{aligned}
D_\alpha D_\beta V^\gamma \quad &= \quad \perp^\mu{}_\alpha \perp^\nu{}_\beta \perp^\gamma{}_\rho \left[(\nabla_\sigma V^\lambda)\perp^\rho{}_\lambda \nabla_\mu \perp^\sigma{}_\nu + (\nabla_\sigma V^\lambda)\perp^\sigma{}_\nu \nabla_\mu \perp^\rho{}_\lambda + \perp^\sigma{}_\nu \perp^\rho{}_\lambda \nabla_\mu \nabla_\sigma V^\lambda\right] \\
&\overset{(F.35)}{=} \quad \perp^\mu{}_\alpha \perp^\nu{}_\beta \perp^\gamma{}_\rho \Big[0 + (\nabla_\sigma V^\lambda)\perp^\rho{}_\lambda n^\sigma \nabla_\mu n_\nu + \underbrace{(\nabla_\sigma V^\lambda) n_\lambda}_{=-V^\lambda \nabla_\sigma n_\lambda} \perp^\sigma{}_\nu \nabla_\mu n^\rho + 0 + \perp^\sigma{}_\nu \perp^\rho{}_\lambda \nabla_\mu \nabla_\sigma V^\lambda\Big] \\
&= \quad \perp^\mu{}_\alpha \perp^\nu{}_\beta \perp^\gamma{}_\lambda n^\sigma (\nabla_\sigma V^\lambda) \nabla_\mu n_\nu - \perp^\mu{}_\alpha \perp^\sigma{}_\beta \perp^\gamma{}_\rho (\nabla_\mu n^\rho) V^\lambda \nabla_\sigma n_\lambda + \perp^\mu{}_\alpha \perp^\sigma{}_\beta \perp^\gamma{}_\lambda \nabla_\mu \nabla_\sigma V^\lambda \\
&= \quad -K_{\alpha\beta} \perp^\gamma{}_\lambda n^\sigma \nabla_\sigma V^\lambda - K_\alpha{}^\gamma K_{\beta\lambda} V^\lambda + \perp^\mu{}_\alpha \perp^\sigma{}_\beta \perp^\gamma{}_\lambda \nabla_\mu \nabla_\sigma V^\lambda \,.
\end{aligned}$$

For the Ricci identity we antisymmetrize over α and β which eliminates the first term,

$$\begin{aligned}
D_\alpha D_\beta V^\gamma - D_\beta D_\alpha V^\gamma \quad &= \quad (K_{\alpha\lambda} K_\beta{}^\gamma - K_{\beta\lambda} K_\alpha{}^\gamma) V^\lambda + \perp^\mu{}_\alpha \perp^\sigma{}_\beta \perp^\gamma{}_\lambda (\nabla_\mu \nabla_\sigma V^\lambda - \nabla_\sigma \nabla_\mu V^\lambda) \\
&= \quad (K_{\alpha\lambda} K_\beta{}^\gamma - K_{\beta\lambda} K_\alpha{}^\gamma) V^\lambda + \perp^\mu{}_\alpha \perp^\sigma{}_\beta \perp^\gamma{}_\lambda R^\lambda{}_{\rho\mu\sigma} V^\rho \\
&\overset{!}{=} \quad \mathcal{R}^\gamma{}_{\rho\alpha\beta} V^\rho \,,
\end{aligned} \tag{F.36}$$

where in the last two lines we have used the four- and three-dimensional Ricci identities. Since $V^\rho = \perp^\rho{}_\sigma V^\sigma$, we find

$$\mathcal{R}^\gamma{}_{\sigma\alpha\beta} V^\sigma = \left[K_{\alpha\rho} K_\beta{}^\gamma - K_{\beta\rho} K_\alpha{}^\gamma + \perp^\mu{}_\alpha \perp^\nu{}_\beta \perp^\gamma{}_\lambda R^\lambda{}_{\rho\mu\nu}\right] \perp^\rho{}_\sigma V^\sigma \,. \tag{F.37}$$

Since this holds for arbitrary spatial vectors V^σ, we get the Gauss equation,

$$\perp^\mu{}_\alpha \perp^\nu{}_\beta \perp^\gamma{}_\lambda \perp^\rho{}_\sigma R^\lambda{}_{\rho\mu\nu} = \perp R^\gamma{}_{\sigma\alpha\beta} = \mathcal{R}^\gamma{}_{\sigma\alpha\beta} + K^\gamma{}_\alpha K_{\beta\sigma} - K^\gamma{}_\beta K_{\alpha\sigma} \,. \tag{F.38}$$

The contracted Gauss equation is obtained by contracting over γ and α,

$$\perp^\nu{}_\beta \perp^\mu{}_\lambda \perp^\rho{}_\sigma R^\lambda{}_{\rho\mu\nu} = \mathcal{R}_{\sigma\beta} + K K_{\beta\sigma} - K^\gamma{}_\beta K_{\gamma\sigma} \qquad \Big| \quad \perp^\mu{}_\lambda = \delta^\mu{}_\lambda + n^\mu n_\lambda$$

$$\Rightarrow \quad \perp^\nu{}_\beta \perp^\rho{}_\sigma R_{\rho\nu} + \perp^\nu{}_\beta \perp^\rho{}_\sigma n^\mu n^\lambda \underbrace{R_{\lambda\rho\mu\nu}}_{=R_{\rho\lambda\nu\mu}} = \mathcal{R}_{\sigma\beta} + K K_{\beta\sigma} - K^\gamma{}_\beta K_{\gamma\sigma} \,, \tag{F.39}$$

or, renaming indices,

$$\perp^\nu{}_\beta \perp^\mu{}_\alpha R_{\mu\nu} + \perp^\rho{}_\beta \perp^\mu{}_\alpha n^\sigma n^\nu R_{\mu\nu\rho\sigma} = \mathcal{R}_{\alpha\beta} + K K_{\alpha\beta} - K_{\alpha\gamma} K^\gamma{}_\beta \,, \tag{F.40}$$

Multiplying with $\gamma^{\alpha\beta} = \perp^{\alpha\beta}$ gives us the scalar version,

$$\gamma^{\mu\nu} R_{\mu\nu} + \gamma^{\mu\rho} n^\sigma n^\nu R_{\mu\nu\rho\sigma} = \mathcal{R} + K^2 - K_{\alpha\gamma} K^{\gamma\alpha}$$

$$\Rightarrow \quad R + n^\mu n^\nu R_{\mu\nu} + g^{\mu\rho} n^\nu n^\sigma R_{\mu\nu\rho\sigma} + \underbrace{n^\mu n^\rho n^\nu n^\sigma R_{\mu\nu\rho\sigma}}_{=0} = \mathcal{R} + K^2 - K^{\mu\nu} K_{\mu\nu}$$

$$\Rightarrow \quad R + 2n^\mu n^\nu R_{\mu\nu} = \mathcal{R} + K^2 - K^{\mu\nu} K_{\mu\nu} \,. \tag{F.41}$$

□

Proposition: The mixed space-time projection of the four-dimensional Riemann tensor is given by the Codazzi equation

$$\perp^\rho{}_\alpha \perp^\sigma{}_\beta \perp^\gamma{}_\mu n^\nu R^\mu{}_{\nu\rho\sigma} = D_\beta K_\alpha{}^\gamma - D_\alpha K_\beta{}^\gamma \,. \tag{F.42}$$

The contracted Codazzi equation is

$$\perp^\mu{}_\alpha n^\nu R_{\mu\nu} = D_\alpha K - D_\mu K_\alpha{}^\mu \,. \tag{F.43}$$

Proof. We apply the four-dimensional Ricci identity to the unit normal vector n^μ and project on all three free indices, which gives us

$$\perp(\nabla_\alpha \nabla_\beta - \nabla_\beta \nabla_\alpha) n^\gamma = \perp R^\gamma{}_{\mu\alpha\beta} n^\mu$$

$$\Rightarrow \quad \perp^\rho{}_\alpha \perp^\sigma{}_\beta \perp^\gamma{}_\tau R^\tau{}_{\mu\rho\sigma} n^\mu = \perp^\rho{}_\alpha \perp^\sigma{}_\beta \perp^\gamma{}_\tau (\nabla_\rho \nabla_\sigma - \nabla_\sigma \nabla_\rho) n^\tau \,. \tag{F.44}$$

Next we recall Eq. (F.9) for the extrinsic curvature, $K_{\alpha\beta} = -\nabla_\alpha n_\beta - n_\alpha a_\beta$, which enables us to write the second derivative of the unit normal as

$$\begin{aligned}
\perp^\rho{}_\alpha \perp^\sigma{}_\beta \perp^\gamma{}_\tau \nabla_\rho \nabla_\sigma n^\tau &= \perp^\rho{}_\alpha \perp^\sigma{}_\beta \perp^\gamma{}_\tau \nabla_\rho (-K_\sigma{}^\tau - n_\sigma a^\tau) \\
&= -\perp^\rho{}_\alpha \perp^\sigma{}_\beta \perp^\gamma{}_\tau (\nabla_\rho K_\sigma{}^\tau + n_\sigma \nabla_\rho a^\tau + a^\tau \nabla_\rho n_\sigma) \\
&= -D_\alpha K_\beta{}^\gamma - a^\gamma \underbrace{\perp^\rho{}_\alpha \perp^\sigma{}_\beta \nabla_\rho n_\sigma}_{=-K_{\alpha\beta}} \,.
\end{aligned} \tag{F.45}$$

The projection of the Riemann tensor is given by the antisymmetrized version of this expression which eliminates the $K_{\alpha\beta}$ term,

$$\perp^\rho{}_\alpha \perp^\sigma{}_\beta \perp^\gamma{}_\tau R^\tau{}_{\mu\rho\sigma} n^\mu = D_\beta K_\alpha{}^\gamma - D_\alpha K_\beta{}^\gamma \,. \tag{F.46}$$

Next, we contract on γ and α,

$$\perp^\rho{}_\gamma \perp^\sigma{}_\beta \perp^\gamma{}_\tau n^\mu R^\tau{}_{\mu\rho\sigma} = D_\beta K - D_\gamma K_\beta{}^\gamma$$

$$\Rightarrow \quad \perp^\rho{}_\tau \perp^\sigma{}_\beta n^\mu R^\tau{}_{\mu\rho\sigma} = (\delta^\rho{}_\tau + n^\rho n_\tau) \perp^\sigma{}_\beta n^\mu R^\tau{}_{\mu\rho\sigma} = \perp^\sigma{}_\beta n^\mu \underbrace{R_{\mu\sigma}}_{=R_{\sigma\mu}} + 0 = D_\beta K - D_\gamma K_\beta{}^\gamma \,.$$

□

The Gauss and Codazzi equations (F.32) and (F.42) have given us two projections of the four-dimensional Riemann tensor, the former with all indices projected onto Σ and the latter with three spatial projections and one onto the timelike unit normal $\boldsymbol{n}$. There is exactly one projection left, that with two spatial and two time projections on the index pairs 1,3 and 2,4 respectively. All other projections result in zero due to the symmetry of the Riemann tensor. For this final projection of the Riemann tensor, it turns out helpful to derive the following auxiliary results.

Lemma :

$$\mathcal{L}_{\boldsymbol{n}}\perp^{\alpha\beta} = n^\alpha a^\beta + n^\beta a^\alpha + 2K^{\alpha\beta}\,, \tag{F.47}$$

$$\mathcal{L}_{\boldsymbol{n}}\perp^{\alpha}{}_{\beta} = n^\alpha a_\beta\,, \tag{F.48}$$

$$\mathcal{L}_{\boldsymbol{n}}\perp_{\alpha\beta} = -2K_{\alpha\beta}\,, \tag{F.49}$$

where $\mathcal{L}_{\boldsymbol{n}}$ denotes the Lie derivative along the unit normal $\boldsymbol{n}$. This implies that for any spatial tensor $T_{\alpha\beta} = \perp T_{\alpha\beta}$,

$$\mathcal{L}_{\boldsymbol{n}}T_{\alpha\beta} = \perp^{\mu}{}_{\alpha}\perp^{\nu}{}_{\beta}\mathcal{L}_{\boldsymbol{n}}T_{\mu\nu}\,, \tag{F.50}$$

i.e. the Lie derivative along $\boldsymbol{n}$ is also spatial. Note that this does in general not hold for upstairs indices as in $\mathcal{L}_{\boldsymbol{n}}T^{\alpha}{}_{\beta}$.
The acceleration vector can be expressed in terms of the lapse function,

$$a_\mu = D_\mu \ln\alpha\,. \tag{F.51}$$

Proof. The first three results follow from the definition of the Lie derivative,

$$\begin{aligned}
\mathcal{L}_{\boldsymbol{n}}\perp^{\alpha\beta} &= n^\mu\nabla_\mu\perp^{\alpha\beta} - \perp^{\mu\beta}\nabla_\mu n^\alpha - \perp^{\alpha\mu}\nabla_\mu n^\beta \\
&= n^\mu\nabla_\mu(n^\alpha n^\beta) + K^{\beta\alpha} + K^{\alpha\beta} \\
&= n^\alpha a^\beta + n^\beta a^\alpha + 2K^{\alpha\beta}\,.
\end{aligned} \tag{F.52}$$

Likewise,

$$\begin{aligned}
\mathcal{L}_{\boldsymbol{n}}\perp^{\alpha}{}_{\beta} &= n^\mu\nabla_\mu\perp^{\alpha}{}_{\beta} - \perp^{\mu}{}_{\beta}\nabla_\mu n^\alpha + \perp^{\alpha}{}_{\mu}\nabla_\beta n^\mu \\
&= n^\mu\nabla_\mu(n^\alpha n_\beta) - \nabla_\beta n^\alpha - n^\mu n_\beta\nabla_\mu n^\alpha + \nabla_\beta n^\alpha + n^\alpha\underbrace{n_\mu\nabla_\beta n^\mu}_{=0} \\
&= n^\alpha a_\beta + n_\beta a^\alpha - n_\beta a^\alpha \;=\; n^\alpha a_\beta\,,
\end{aligned} \tag{F.53}$$

and

$$\mathcal{L}_{\boldsymbol{n}}\perp_{\alpha\beta} = n^\mu\nabla_\mu\perp_{\alpha\beta} + \perp_{\mu\beta}\nabla_\alpha n^\mu + \perp_{\alpha\mu}\nabla_\beta n^\mu = n^\mu\nabla_\mu(n_\alpha n_\beta) + g_{\mu\beta}\nabla_\alpha n^\mu + g_{\alpha\mu}\nabla_\beta n^\mu$$

$$
\begin{aligned}
&= n^\mu n_\beta \nabla_\mu n_\alpha + n^\mu n_\alpha \nabla_\mu n_\beta + \nabla_\alpha n_\beta + \nabla_\beta n_\alpha \\
&= (\delta^\mu{}_\alpha + n^\mu n_\alpha)\nabla_\mu n_\beta + (\delta^\mu{}_\beta + n^\mu n_\beta)\nabla_\mu n_\alpha \\
&= \perp^\mu{}_\alpha \nabla_\mu n_\beta + \perp^\mu{}_\beta \nabla_\mu n_\alpha \;=\; -K_{\alpha\beta} - K_{\beta\alpha} \;=\; -2K_{\alpha\beta}\,. \qquad \text{(F.54)}
\end{aligned}
$$

With the Lie derivatives of the projector, we find that a spatial tensor $T_{\alpha\beta}$ satisfies

$$
\begin{aligned}
\mathcal{L}_{\boldsymbol{n}} T_{\alpha\beta} &= \mathcal{L}_{\boldsymbol{n}}(\perp^\mu{}_\alpha \perp^\nu{}_\beta T_{\mu\nu}) \;=\; \perp^\mu{}_\alpha \perp^\nu{}_\beta \mathcal{L}_{\boldsymbol{n}} T_{\mu\nu} + \perp^\mu{}_\alpha T_{\mu\nu} \mathcal{L}_{\boldsymbol{n}} \perp^\nu{}_\beta + \perp^\nu{}_\beta T_{\mu\nu} \mathcal{L}_{\boldsymbol{n}} \perp^\mu{}_\alpha \\
&= \perp^\mu{}_\alpha \perp^\nu{}_\beta \mathcal{L}_{\boldsymbol{n}} T_{\mu\nu} + T_{\alpha\nu} n^\nu a_\beta + T_{\mu\beta} n^\mu a_\alpha \\
&= \perp^\mu{}_\alpha \perp^\nu{}_\beta \mathcal{L}_{\boldsymbol{n}} T_{\mu\nu}\,, \qquad \text{(F.55)}
\end{aligned}
$$

since $T_{\alpha\mu} n^\mu = 0$.

For the acceleration vector, we use the definition of the unit vector, $\boldsymbol{n} = -\alpha \mathbf{d}t \Leftrightarrow n_\mu = -\alpha \nabla_\mu t$ from Eq. (F.1). Furthermore, our connection is torsion free, so that second covariant derivatives of scalars commute. This gives us

$$
\begin{aligned}
a_\beta &= n^\mu \nabla_\mu n_\beta \;=\; -n^\mu \nabla_\mu (\alpha \nabla_\beta t) \;=\; -\alpha n^\mu \underbrace{\nabla_\mu \nabla_\beta t}_{\nabla_\beta \nabla_\mu t} - n^\mu \underbrace{(\nabla_\beta t)}_{=-\frac{1}{\alpha} n_\beta} \nabla_\mu \alpha \\
&= \alpha n^\mu \nabla_\beta \frac{n_\mu}{\alpha} + \frac{n^\mu n_\beta}{\alpha} \nabla_\mu \alpha \;=\; \underbrace{n^\mu \nabla_\beta n_\mu}_{=0} - \alpha n^\mu n_\mu \frac{\nabla_\beta \alpha}{\alpha^2} + \frac{n^\mu n_\beta}{\alpha} \nabla_\mu \alpha \\
&= \frac{1}{\alpha}\Big(\delta^\mu{}_\beta \nabla_\mu \alpha + n^\mu n_\beta \nabla_\mu \alpha\Big) \;=\; \perp^\mu{}_\beta \frac{\nabla_\mu \alpha}{\alpha} \;=\; \frac{D_\beta \alpha}{\alpha} \;=\; D_\beta \ln \alpha\,. \qquad \text{(F.56)}
\end{aligned}
$$

□

Proposition: The space-time-space-time projection of the Riemann tensor is given by the Ricci equation (not to be confused with the Ricci identity),

$$
\perp^\mu{}_\alpha n^\nu \perp^\rho{}_\gamma n^\sigma R_{\mu\nu\rho\sigma} = \mathcal{L}_{\boldsymbol{n}} K_{\alpha\gamma} + \frac{1}{\alpha} D_\alpha D_\gamma \alpha + K_{\rho\gamma} K_\alpha{}^\rho\,. \qquad \text{(F.57)}
$$

Proof. We start with the four-dimensional Ricci identity applied to the unit normal n^μ,

$$
\nabla_\rho \nabla_\sigma n^\mu - \nabla_\sigma \nabla_\rho n^\mu = R^\mu{}_{\nu\rho\sigma} n^\nu\,. \qquad \text{(F.58)}
$$

Projecting this equation twice onto space and once onto time gives us

$$
\begin{aligned}
\perp_{\alpha\mu} n^\nu \perp^\rho{}_\gamma n^\sigma R^\mu{}_{\nu\rho\sigma} &= \perp_{\alpha\mu} \perp^\rho{}_\gamma n^\sigma (\nabla_\rho \nabla_\sigma n^\mu - \nabla_\sigma \nabla_\rho n^\mu) \qquad \Big|\; K_{\alpha\beta} = -\nabla_\alpha n_\beta - n_\alpha a_\beta \\
&= \perp_{\alpha\mu} \perp^\rho{}_\gamma n^\sigma \Big[\nabla_\rho(-K_\sigma{}^\mu - n_\sigma a^\mu) + \nabla_\sigma (K_\rho{}^\mu + n_\rho a^\mu)\Big]
\end{aligned}
$$

$$
\begin{aligned}
&= \perp_{\alpha\mu}\perp^{\rho}{}_{\gamma} n^{\sigma}\Big[-\nabla_{\rho}K_{\sigma}{}^{\mu} - a^{\mu}\nabla_{\rho}n_{\sigma} - n_{\sigma}\nabla_{\rho}a^{\mu} + \nabla_{\sigma}K_{\rho}{}^{\mu} + a^{\mu}\nabla_{\sigma}n_{\rho} + n_{\rho}\nabla_{\sigma}a^{\mu}\Big] \\
&= \perp_{\alpha\mu}\perp^{\rho}{}_{\gamma}\Big[K^{\mu}{}_{\sigma}\nabla_{\rho}n^{\sigma} - 0 + \nabla_{\rho}a^{\mu} + n^{\sigma}\nabla_{\sigma}K_{\rho}{}^{\mu} + a^{\mu}a_{\rho} + 0\Big] \\
&= K_{\alpha\sigma}(-K_{\gamma}{}^{\sigma}) + D_{\gamma}a_{\alpha} + \perp_{\alpha}{}^{\mu}\perp^{\rho}{}_{\gamma}n^{\sigma}\nabla_{\sigma}K_{\rho\mu} + a_{\alpha}a_{\gamma} \\
&= -K_{\alpha\sigma}K^{\sigma}{}_{\gamma} + D_{\gamma}a_{\alpha} + a_{\alpha}a_{\gamma} + \perp^{\mu}{}_{\alpha}\perp^{\rho}{}_{\gamma}n^{\sigma}\nabla_{\sigma}K_{\rho\mu}\,, \qquad \text{(F.59)}
\end{aligned}
$$

where we have used $n_{\mu}K^{\mu}{}_{\sigma} = 0$ to trade ∇K for ∇n, and $n^{\sigma}\nabla_{\rho}n_{\sigma} = 0$.

The next step in our proof consists in expressing the covariant derivative of the extrinsic curvature in terms of the Lie derivative along $\boldsymbol{n}$. For this purpose, we apply the Lemma (F.50) to the extrinsic curvature which is spatial in both indices,

$$
\begin{aligned}
\mathcal{L}_{\boldsymbol{n}}K_{\alpha\beta} &= \perp^{\mu}{}_{\alpha}\perp^{\nu}{}_{\beta}\mathcal{L}_{\boldsymbol{n}}K_{\mu\nu} = \perp^{\mu}{}_{\alpha}\perp^{\nu}{}_{\beta}\Big[n^{\rho}\nabla_{\rho}K_{\mu\nu} + K_{\rho\nu}\nabla_{\mu}n^{\rho} + K_{\mu\rho}\nabla_{\nu}n^{\rho}\Big] \\
\Rightarrow\ \perp^{\mu}{}_{\alpha}\perp^{\nu}{}_{\beta}n^{\sigma}\nabla_{\sigma}K_{\mu\nu} &= \mathcal{L}_{\boldsymbol{n}}K_{\alpha\beta} - K_{\rho\beta}\perp^{\mu}{}_{\alpha}\nabla_{\mu}n^{\rho} - K_{\alpha\rho}\perp^{\nu}{}_{\beta}\nabla_{\nu}n^{\rho} \\
&= \mathcal{L}_{\boldsymbol{n}}K_{\alpha\beta} + K_{\rho\beta}K_{\alpha}{}^{\rho} + K_{\alpha\rho}K_{\beta}{}^{\rho}\,. \qquad \text{(F.60)}
\end{aligned}
$$

We use this result to substitute for the last term in Eq. (F.59), so that

$$
\begin{aligned}
\perp_{\alpha\mu}n^{\nu}\perp^{\rho}{}_{\gamma}n^{\sigma}R^{\mu}{}_{\nu\rho\sigma} &= -\underset{\sim\sim\sim}{K_{\alpha\sigma}K^{\sigma}{}_{\gamma}} + D_{\gamma}a_{\alpha} + a_{\alpha}a_{\gamma} + \mathcal{L}_{\boldsymbol{n}}K_{\alpha\gamma} + K_{\rho\gamma}K_{\alpha}{}^{\rho} + \underset{\sim\sim\sim}{K_{\alpha\rho}K_{\gamma}{}^{\rho}} \\
&= \mathcal{L}_{\boldsymbol{n}}K_{\alpha\gamma} + D_{\gamma}a_{\alpha} + a_{\alpha}a_{\gamma} + K_{\rho\gamma}K_{\alpha}{}^{\rho}\,. \qquad \text{(F.61)}
\end{aligned}
$$

Finally, we substitute for the acceleration terms using[9] Eq. (F.51),

$$
\begin{aligned}
D_{\beta}a_{\alpha} + a_{\alpha}a_{\beta} &= D_{\beta}\frac{D_{\alpha}\alpha}{\alpha} + \frac{D_{\alpha}\alpha}{\alpha}\frac{D_{\beta}\alpha}{\alpha} = \frac{1}{\alpha}D_{\beta}D_{\alpha}\alpha - (D_{\alpha}\alpha)\frac{D_{\beta}\alpha}{\alpha^2} + \frac{(D_{\alpha}\alpha)(D_{\beta}\alpha)}{\alpha^2} \\
&= \frac{1}{\alpha}D_{\beta}D_{\alpha}\alpha = \frac{1}{\alpha}D_{\alpha}D_{\beta}\alpha\,, \qquad \text{(F.62)}
\end{aligned}
$$

where the last equality follows from the torsion free nature of D_{μ}. □

The Gauss, Codazzi and Ricci equations and their contractions enable us to express the four-dimensional Ricci tensor and scalar exclusively in terms of 3+1 variables.

Proposition: The four-dimensional Ricci tensor and scalar satisfy the relations

$$
\begin{aligned}
\perp^{\mu}{}_{\alpha}\perp^{\nu}{}_{\beta}R_{\mu\nu} &= -\mathcal{L}_{\boldsymbol{n}}K_{\alpha\beta} - \frac{1}{\alpha}D_{\alpha}D_{\beta}\alpha - 2K_{\alpha\rho}K^{\rho}{}_{\beta} + \mathcal{R}_{\alpha\beta} + KK_{\alpha\beta}\,, \\
R &= -2\mathcal{L}_{\boldsymbol{n}}K - \frac{2}{\alpha}D^{\mu}D_{\mu}\alpha + \mathcal{R} + K^2 + K_{\mu\nu}K^{\mu\nu}\,. \qquad \text{(F.63)}
\end{aligned}
$$

[9]It is unfortunate that the letter α appears here with two meanings, first as an index and second as the lapse function. An alternative notation found in the literature uses N for the lapse function and N^i for the shift vector – which we will define shortly. This double usage of N does not appear too much of an improvement, though, and we will use the more common α for the lapse and β^i for the shift vector.

Proof. The contracted Gauss equation (F.33) gave us

$$\perp^{\mu}{}_{\alpha}\perp^{\nu}{}_{\beta}R_{\mu\nu} + \perp^{\mu}{}_{\alpha}\perp^{\rho}{}_{\beta}n^{\nu}n^{\sigma}R_{\mu\nu\rho\sigma} = \mathcal{R}_{\alpha\beta} + KK_{\alpha\beta} - K_{\alpha\mu}K^{\mu}{}_{\beta}\,,$$

which we can combine with the Ricci equation (F.57) where we place γ by β,

$$\perp^{\mu}{}_{\alpha}n^{\nu}\perp^{\rho}{}_{\beta}n^{\sigma}R_{\mu\nu\rho\sigma} = \mathcal{L}_{\boldsymbol{n}}K_{\alpha\beta} + \frac{1}{\alpha}D_{\alpha}D_{\beta}\alpha + K_{\rho\beta}K_{\alpha}{}^{\rho}\,,$$

such that

$$\perp^{\mu}{}_{\alpha}\perp^{\nu}{}_{\beta}R_{\mu\nu} = -\mathcal{L}_{\boldsymbol{n}}K_{\alpha\beta} - \frac{1}{\alpha}D_{\alpha}D_{\beta}\alpha - 2K_{\alpha\rho}K^{\rho}{}_{\beta} + \mathcal{R}_{\alpha\beta} + KK_{\alpha\beta}\,. \tag{F.64}$$

This is our first result. For the second we use our Lemma (F.47) to obtain

$$\perp^{\alpha\beta}\mathcal{L}_{\boldsymbol{n}}K_{\alpha\beta} = \mathcal{L}_{\boldsymbol{n}}K - K_{\alpha\beta}\mathcal{L}_{\boldsymbol{n}}\perp^{\alpha\beta} = \mathcal{L}_{\boldsymbol{n}}K - K_{\alpha\beta}\Big[n^{\alpha}a^{\beta} + n^{\beta}a^{\alpha} + 2K^{\alpha\beta}\Big] = \mathcal{L}_{\boldsymbol{n}}K - 2K_{\alpha\beta}K^{\alpha\beta}\,,$$

since $K_{\alpha\mu}n^{\mu} = 0$. Next, we contract Eq. (F.64) with $\perp^{\alpha\beta}$,

$$\perp^{\alpha\beta}\perp^{\mu}{}_{\alpha}\perp^{\nu}{}_{\beta}R_{\mu\nu} = -\mathcal{L}_{\boldsymbol{n}}K + 2K_{\alpha\beta}K^{\alpha\beta} - \frac{1}{\alpha}\perp^{\alpha\beta}D_{\alpha}D_{\beta}\alpha - 2K_{\alpha\rho}K^{\alpha\rho} + \mathcal{R} + K^{2}$$

$$\Rightarrow \quad R + n^{\mu}n^{\nu}R_{\mu\nu} = -\mathcal{L}_{\boldsymbol{n}}K - \frac{1}{\alpha}D^{\mu}D_{\mu}\alpha + \mathcal{R} + K^{2}\,. \tag{F.65}$$

This can be combined with the scalar Gauss equation (F.33)

$$R + 2n^{\mu}n^{\nu}R_{\mu\nu} = \mathcal{R} + K^{2} - K_{\mu\nu}K^{\mu\nu}\,,$$

which leads to

$$R = -2\mathcal{L}_{\boldsymbol{n}}K - \frac{2}{\alpha}D^{\mu}D_{\mu}\alpha + \mathcal{R} + K^{2} + K_{\mu\nu}K^{\mu\nu}\,. \tag{F.66}$$

We could similarly express $n^{\mu}n^{\nu}R_{\mu\nu}$ in terms of 3+1 variables, but as it will turn out, we have this time-time projection in exactly the required from already in the scalar Gauss equation (F.33). Finally, the mixed projection $\perp n^{\mu}R_{\alpha\mu}$ is already given by the contracted Codazzi equation (F.43). □

F.4 The 3+1 version of the Einstein equations

We now turn our attention to the projections of the Einstein equations which we will consider in two forms, (i) Eq. (A.4) with the Einstein tensor expanded in terms of the Ricci tensor, and (ii) the trace reversed form. For completeness, we will also add the cosmological constant Λ,

$$R_{\alpha\beta} - \frac{1}{2}Rg_{\alpha\beta} + \Lambda g_{\alpha\beta} = 8\pi T_{\alpha\beta} \qquad \Leftrightarrow \qquad R_{\alpha\beta} = 8\pi\left(T_{\alpha\beta} - \frac{1}{2}Tg_{\alpha\beta}\right) + \Lambda g_{\alpha\beta}\,, \tag{F.67}$$

where $T \coloneqq T^{\mu}{}_{\mu}$. Here we have used that the trace of the first version is given by

$$-R + 4\Lambda = 8\pi T \qquad \Rightarrow \qquad \frac{1}{2}R = 2\Lambda - \frac{1}{2}8\pi T\,. \tag{F.68}$$

For projecting the equations, we define the 3+1 decomposition of the energy momentum tensor.

Def. : The *energy density*, *momentum density* and *stress tensor* are defined by

$$\rho := n^\mu n^\nu T_{\mu\nu}\,, \qquad j_\alpha := -\perp^\mu{}_\alpha n^\nu T_{\mu\nu}\,, \qquad S_{\alpha\beta} := \perp^\mu{}_\alpha \perp^\nu{}_\beta T_{\mu\nu}$$

$$\Rightarrow \quad T_{\alpha\beta} = \rho n_\alpha n_\beta + j_\alpha n_\beta + n_\alpha j_\beta + S_{\alpha\beta}\,. \tag{F.69}$$

A quick calculation shows that the trace T can be written as

$$T = g^{\mu\nu}T_{\mu\nu} = -\rho - 0 - 0 + g^{\mu\nu}S_{\mu\nu} = -\rho + (\gamma^{\mu\nu} - n^\mu n^\nu)S_{\mu\nu} = -\rho + S - 0 = S - \rho\,. \tag{F.70}$$

Now let's project...

Proposition: The time-time, space-time and space-space projections of the Einstein equations are

$$\mathcal{H} \quad := \quad \mathcal{R} + K^2 - K_{\mu\nu}K^{\mu\nu} - 2\Lambda - 16\pi\rho = 0\,, \tag{F.71}$$

$$\mathcal{M}_\alpha \quad := \quad D_\alpha K - D_\mu K_\alpha{}^\mu + 8\pi j_\alpha = 0\,, \tag{F.72}$$

$$\mathcal{L}_{\boldsymbol{n}}\gamma_{\alpha\beta} \quad = \quad -2K_{\alpha\beta}\,, \tag{F.73}$$

$$\begin{aligned} \mathcal{L}_{\boldsymbol{n}}K_{\alpha\beta} \quad &= \quad -\frac{1}{\alpha}D_\alpha D_\beta \alpha - 2K_{\alpha\mu}K^\mu{}_\beta + \mathcal{R}_{\alpha\beta} + KK_{\alpha\beta} - \Lambda\gamma_{\alpha\beta} \\ &\quad\quad -8\pi\left[S_{\alpha\beta} - \frac{1}{2}\gamma_{\alpha\beta}(S-\rho)\right]\,. \end{aligned} \tag{F.74}$$

The first two are commonly referred to as the *Hamiltonian constraint* and the *momentum constraints*. The third and fourth equations contain Lie derivatives along $\boldsymbol{n}$ which represent time derivatives. These equations constitute a first-order system for a second-order in time evolution of the spatial metric $\gamma_{\alpha\beta}$ with the extrinsic curvature playing the role of an auxiliary variable.

Proof. Let us start with the Hamiltonian constraint. We project the first version of the Einstein equation (F.67) twice onto time and use the scalar Gauss equation (F.33)

$$n^\alpha n^\beta R_{\alpha\beta} + \frac{1}{2}R - \Lambda = 8\pi\rho$$

$$\Rightarrow \quad R + 2n^\alpha n^\beta R_{\alpha\beta} - 2\Lambda = 16\pi\rho$$

$$\overset{(F.33)}{\Rightarrow} \quad \mathcal{R} + K^2 - K^{\mu\nu}K_{\mu\nu} - 2\Lambda - 16\pi\rho = 0\,. \tag{F.75}$$

Next, we project the first version of the Einstein equation (F.67) once onto space and once onto time and use the contracted Codazzi equation (F.43),

$$\begin{aligned}
&\perp^\mu{}_\alpha n^\nu R_{\mu\nu} - \frac{1}{2}\underbrace{g_{\mu\nu}\perp^\mu{}_\alpha n^\nu}_{=0} R + \Lambda g_{\mu\nu}\perp^\mu{}_\alpha n^\nu = 8\pi \perp^\mu{}_\alpha n^\nu T_{\mu\nu} \\
\Rightarrow\quad &\perp^\mu{}_\alpha n^\nu R_{\mu\nu} = -8\pi j_\alpha \\
\overset{(F.43)}{\Rightarrow}\quad & D_\alpha K - D_\mu K_\alpha{}^\mu + 8\pi j_\alpha = 0\,. \qquad \text{(F.76)}
\end{aligned}$$

The third equation (F.73) in our above set is Eq. (F.49) and has already been derived there. Finally, we project the trace-reversed version of the Einstein equation (F.67) twice onto space and use the first relation in (F.63), and thus obtain

$$\begin{aligned}
&\perp^\mu{}_\alpha \perp^\nu{}_\beta R_{\mu\nu} = \Lambda\gamma_{\alpha\beta} + 8\pi\left(S_{\alpha\beta} - \frac{1}{2}\gamma_{\alpha\beta}T\right) \\
\overset{(F.63)}{\Rightarrow}\quad & -\mathcal{L}_{\boldsymbol{n}}K_{\alpha\beta} - \frac{1}{\alpha}D_\alpha D_\beta \alpha - 2K_{\alpha\mu}K^\mu{}_\beta + \mathcal{R}_{\alpha\beta} + KK_{\alpha\beta} = \Lambda\gamma_{\alpha\beta} + 8\pi\left[S_{\alpha\beta} - \frac{1}{2}(S-\rho)\gamma_{\alpha\beta}\right] \\
\Rightarrow\quad & \mathcal{L}_{\boldsymbol{n}}K_{\alpha\beta} = -\frac{1}{\alpha}D_\alpha D_\beta \alpha - 2K_{\alpha\mu}K^\mu{}_\beta + \mathcal{R}_{\alpha\beta} + KK_{\alpha\beta} - \Lambda\gamma_{\alpha\beta} - 8\pi\left[S_{\alpha\beta} - \frac{1}{2}(S-\rho)\gamma_{\alpha\beta}\right]
\end{aligned}$$

□

F.5 Adapted coordinates

Def. : Let $(\mathcal{M}, \boldsymbol{g})$ be a globally hyperbolic spacetime with a foliation Σ_t constructed from a function $t : \mathcal{M} \to \mathbb{R}$ with $\mathbf{d}t \neq 0$ according to the definitions on Page 40. A coordinate system *adapted to the foliation* is a coordinate chart

$$x^\alpha = (t,\, x^i) \quad \text{with} \quad i = 1,\, 2,\, 3\,, \qquad \text{(F.77)}$$

where x^i label points uniquely inside each Σ_t.

Note that adapted coordinates define a coordinate basis $\boldsymbol{\partial}_t,\ \boldsymbol{\partial}_i$ for vectors and $\mathbf{d}t,\ \mathbf{d}x^i$ for one-forms.

Def. : The *shift vector* is defined by

$$\boldsymbol{\beta} := \boldsymbol{\partial}_t - \alpha\boldsymbol{n}\,. \qquad \text{(F.78)}$$

The shift vector is tangent to Σ since

$$\langle \mathbf{d}t, \boldsymbol{\beta}\rangle = \langle \mathbf{d}t, \boldsymbol{\partial}_t\rangle - \alpha\langle \mathbf{d}t, \boldsymbol{n}\rangle = 1 + \langle \boldsymbol{n}, \boldsymbol{n}\rangle = 0\,, \qquad \text{(F.79)}$$

where we have used $\mathbf{d}t = -\alpha\boldsymbol{n}$. The shift vector and its relation to the unit normal $\boldsymbol{n}$ and the coordinate vector $\boldsymbol{\partial}_t$ are graphically illustrated in Fig. 13. There we see that the shift

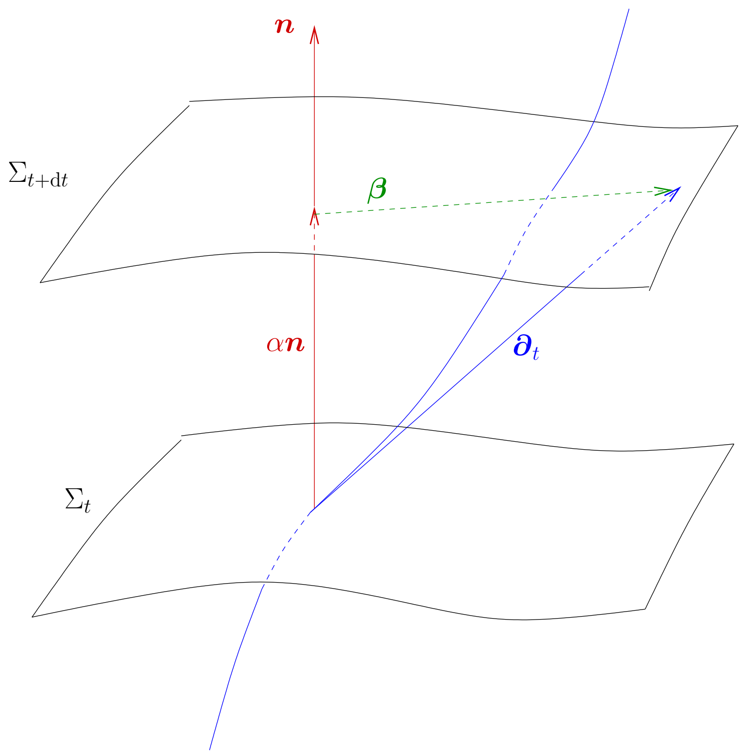


Figure 13: Illustration of a spacetime foliation constructed from hypersurfaces Σ_t, $t \in \mathbb{R}$. Adapted coordinates are given by (t, x^i) where t labels the hypersurface and x^i points inside each Σ_t. The coordinate vector $\boldsymbol{\partial}_t$ is tangent to the curves x^i = const. The shift vector is a measure of this coordinate vector's deviation from the direction normal to the hypersurface given by the unit normal vector $\boldsymbol{n}$.

measures the deviation of the coordinate vector $\boldsymbol{\partial}_t$ from the direction normal to Σ_t. Note that the integral curves of $\boldsymbol{\partial}_t$ are determined by the way we assign spatial coordinates x^i to points inside each hypersurface; their deviation from the normal direction, i.e. the shift vector, is therefore completely coordinate dependent. In other words, the shift encapsulates three of the four gauge or coordinate conditions of general relativity.

The fourth and final degree of gauge freedom is contained in the lapse function α, but that will become clearer after we have discussed how the metric components look like in adapted coordinates. For this purpose we recall that the components of a tensor are obtained by filling its slots with the basis vectors and one-forms. For the metric with downstairs indices, we thus obtain

$$\begin{aligned}
g_{00} &= \boldsymbol{g}(\boldsymbol{\partial}_t, \boldsymbol{\partial}_t) = \boldsymbol{g}(\alpha\boldsymbol{n} + \boldsymbol{\beta}, \alpha\boldsymbol{n} + \boldsymbol{\beta}) = -\alpha^2 + \beta^m \beta_m \,, \\
g_{0i} &= \boldsymbol{g}(\boldsymbol{\partial}_t, \boldsymbol{\partial}_i) = \boldsymbol{g}(\alpha\boldsymbol{n} + \boldsymbol{\beta}, \boldsymbol{\partial}_i) = -\langle \mathbf{d}t, \boldsymbol{\partial}_i \rangle + \langle \beta_m \mathbf{d}x^m, \boldsymbol{\partial}_i \rangle = \beta_i \,, \\
g_{ij} &= \boldsymbol{g}(\boldsymbol{\partial}_i, \boldsymbol{\partial}_j) = \boldsymbol{\gamma}(\boldsymbol{\partial}_i, \boldsymbol{\partial}_j) = \gamma_{ij} \,,
\end{aligned} \tag{F.80}$$

where we have used $\beta^0 = \langle \mathbf{d}t, \boldsymbol{\beta} \rangle = 0$, so that $\beta_m = g_{mn}\beta^n = \gamma_{mn}\beta^n$, and the fact that the vectors $\boldsymbol{\partial}_i$ are spatial by construction, so that $\boldsymbol{g}(\boldsymbol{\partial}_i, \boldsymbol{\partial}_j) = \boldsymbol{\gamma}(\boldsymbol{\partial}_i, \boldsymbol{\partial}_j)$.

Proposition: The components of the spacetime metric $\boldsymbol{g}$ are given by

$$g_{\alpha\beta} = \left(\begin{array}{c|c} -\alpha^2 + \beta^m\beta_m & \beta_j \\ \hline \beta_i & \gamma_{ij} \end{array}\right) \quad \Leftrightarrow \quad g^{\alpha\beta} = \left(\begin{array}{c|c} -\alpha^{-2} & \alpha^{-2}\beta^j \\ \hline \alpha^{-2}\beta^i & \gamma^{ij} - \alpha^{-2}\beta^i\beta^j \end{array}\right)$$

$$\begin{aligned} \Rightarrow \quad \mathrm{d}s^2 &= (-\alpha^2 + \beta_i\beta^i)\mathrm{d}t^2 + 2\beta_i \mathrm{d}t\,\mathrm{d}x^i + \gamma_{ij}\mathrm{d}x^i\,\mathrm{d}x^j \\ &= -\alpha^2\mathrm{d}t^2 + \gamma_{ij}(\mathrm{d}x^i + \beta^i\mathrm{d}t)(\mathrm{d}x^j + \beta^j\mathrm{d}t)\,, \end{aligned} \tag{F.81}$$

where γ^{ij} is defined as the inverse of the 3×3 matrix γ_{ij}. In adapted coordinates, the components of the unit normal vector are

$$n_\alpha = (-\alpha,\, 0)\,, \qquad n^\alpha = \left(\frac{1}{\alpha},\, -\frac{\beta^i}{\alpha}\right)\,. \tag{F.82}$$

Proof. We have already derived the components of the downstairs metric. The upstairs version can be verified either by directly showing $g^{\alpha\mu}g_{\mu\beta} = \delta^\alpha{}_\beta$ or by computing the inverse metric from the cofactor matrices according to the method described on Page 50.

The components of n_α directly follow from the definition $\boldsymbol{n} = -\alpha\mathbf{d}t$. Raising the index with the metric gives us

$$n^\alpha = g^{\alpha\mu}n_\mu = \left[-\alpha^{-2}(-\alpha),\, \alpha^{-2}\beta^i(-\alpha)\right] = \left[\frac{1}{\alpha},\, -\frac{\beta^i}{\alpha}\right]\,. \tag{F.83}$$

□

Proposition: The proper time measured by an observer moving with four-velocity $u^\alpha = n^\alpha$ from hypersurface Σ_t to hypersurface $\Sigma_{t+\mathrm{d}t}$ is

$$\mathrm{d}\tau = \alpha \mathrm{d}t\,. \tag{F.84}$$

Proof. We first note that $n_\mu n^\mu = -1$ and $\boldsymbol{n}$ is timelike, so it is a four-velocity. We parametrize the world line of the observer moving along $\boldsymbol{n}$ with our coordinate time t. The tangent vector to the wordline *with this parametrization* must be proportional to n^α but will in general not be equal to it. Let us call this tangent vector $\boldsymbol{m}$. By definition,

$$m^\alpha = \frac{\mathrm{d}x^\alpha}{\mathrm{d}t} = \left(\frac{\mathrm{d}t}{\mathrm{d}t},\, \frac{\mathrm{d}x^i}{\mathrm{d}t}\right) = \left(1,\, \frac{\mathrm{d}x^i}{\mathrm{d}t}\right) \propto n^\alpha = \left(\frac{1}{\alpha},\, -\frac{\beta^i}{\alpha}\right)$$

$$\Rightarrow \quad m^\alpha = \alpha n^\alpha = \left(1,\, -\beta^i\right)\,.$$

The proper time along the integral curve of m^α is

$$\Delta\tau = \int_{t_1}^{t_2} \sqrt{-g_{\mu\nu}\frac{\mathrm{d}x^\mu}{\mathrm{d}t}\frac{\mathrm{d}x^\nu}{\mathrm{d}t}}\,\mathrm{d}t \qquad \Rightarrow \qquad \mathrm{d}\tau = \sqrt{-g_{\mu\nu}\frac{\mathrm{d}x^\mu}{\mathrm{d}t}\frac{\mathrm{d}x^\nu}{\mathrm{d}t}}\,\mathrm{d}t$$

Using the metric components from Eq. (F.81), this gives us

$$\mathrm{d}\tau = \sqrt{-g_{00}m^0m^0 - 2g_{0i}m^0m^i - g_{ij}m^im^j}\,\mathrm{d}t = \sqrt{\alpha^2 - \beta_m\beta^m - 2\beta_i(-\beta^i) - \gamma_{ij}\beta^i\beta^j}\,\mathrm{d}t = \alpha\mathrm{d}t\,.$$

□

So the lapse function determines the amount of proper time (as measured by normal observers) that separates two infinitesimally close hypersurfaces Σ_t and $\Sigma_{t+\mathrm{d}t}$. This amount of proper time clearly depends on the way we label the hypersurfaces or how we *slice* the spacetime; for example, doubling the coordinate time value of every slice, $t \to \tilde{t} = 2t$, will double the proper time separating two infinitesimally close hypersurfaces $\Sigma_{\tilde{t}}$ and $\Sigma_{\tilde{t}+\mathrm{d}\tilde{t}}$. In summary, the shift vector β^i determines our choice of spatial coordinates x^i and the lapse function determines our choice of the time coordinate t. Lapse and shift thus encapsulate the gauge freedom of general relativity.

Adapted coordinates also enable us to formulate equations for spatial objects in terms of three-dimensional geometry using Latin indices $i, j, \ldots = 1, 2, 3$. Consider, for example, a vector V^α tangent to Σ. In adapted coordinates, we find

$$V^0 = \boldsymbol{V}(\mathbf{d}x^0) = \boldsymbol{V}(\mathbf{d}t) = \langle \mathbf{d}t, \boldsymbol{V}\rangle = 0\,, \tag{F.85}$$

so the vector is completely determined by its three spatial components V^i. By the same argument, any tensor component with one upstairs index 0 vanishes, e.g. $T^{0\beta}{}_{\mu\nu} = 0$. In general, this does not hold for downstairs indices; for example,

$$V_0 = g_{0\mu}V^\mu = g_{0i}V^i = \beta_iV^i\,, \tag{F.86}$$

is in general non-zero. Even in that case, however, the component V_0 does not contain any independent information, since all four components V_α are determined by the three V^i (and the spacetime metric). Furthermore, any contraction of indices acquires non-zero contributions only from the spatial contraction, e.g.

$$V^\mu T_{\mu\alpha} = \underbrace{V^0}_{=0} T_{0\alpha} + V^m T_{m\alpha} = V^m T_{m\alpha}\,. \tag{F.87}$$

In adapted coordinates, we can therefore replace in equations for spatial objects all Greek indices with Latin indices. In particular, this applies to our 3+1 decomposition of the Einstein equations (F.71)-(F.74). Before we do that, however, we derive a convenient expression for the Lie derivatives appearing in these equations.

Proposition: In adapted coordinates

$$\mathcal{L}_{\boldsymbol{n}}\gamma_{\mu\nu} = \frac{1}{\alpha}\partial_t\gamma_{\mu\nu} - \frac{1}{\alpha}\mathcal{L}_{\beta}\gamma_{\mu\nu}\,, \tag{F.88}$$

$$\mathcal{L}_{\boldsymbol{n}}K_{\mu\nu} = \frac{1}{\alpha}\partial_t K_{\mu\nu} - \frac{1}{\alpha}\mathcal{L}_{\beta}K_{\mu\nu}\,, \tag{F.89}$$

where $\mathcal{L}_{\beta}$ is the Lie derivative along the shift vector.

Proof. Let $T_{\alpha\beta}$ be a tensor tangent to Σ in both indices, i.e. $T_{\mu\nu}n^{\mu} = 0 = T_{\mu\nu}n^{\nu}$, f be a scalar function and $\boldsymbol{n}$ the timelike unit normal. We then obtain

$$\begin{aligned}
\mathcal{L}_{f\boldsymbol{n}}T_{\alpha\beta} &= fn^{\mu}\nabla_{\mu}T_{\alpha\beta} + T_{\mu\beta}\nabla_{\alpha}(fn^{\mu}) + T_{\alpha\mu}\nabla_{\beta}(fn^{\mu}) \\
&= f\left(n^{\mu}\nabla_{\mu}T_{\alpha\beta} + T_{\mu\beta}\nabla_{\alpha}n^{\mu} + T_{\alpha\mu}\nabla_{\beta}n^{\mu}\right) + \underbrace{T_{\mu\beta}n^{\mu}}_{=0}\nabla_{\alpha}f + \underbrace{T_{\alpha\mu}n^{\mu}}_{=0}\nabla_{\beta}f \\
&= f\mathcal{L}_{\boldsymbol{n}}T_{\alpha\beta}\,.
\end{aligned} \tag{F.90}$$

Writing Eq. (F.82) as $\boldsymbol{n} = \frac{1}{\alpha}(\boldsymbol{\partial}_t - \boldsymbol{\beta})$, and bearing in mind that both $K_{\alpha\beta}$ and $\gamma_{\alpha\beta}$ are spatial in both indices, this result with $f = 1/\alpha$ implies that

$$\mathcal{L}_{\boldsymbol{n}}K_{\mu\nu} = \mathcal{L}_{\frac{1}{\alpha}(\boldsymbol{\partial}_t - \boldsymbol{\beta})}K_{\mu\nu} = \frac{1}{\alpha}\left(\mathcal{L}_{\boldsymbol{\partial}_t}K_{\mu\nu} - \mathcal{L}_{\boldsymbol{\beta}}K_{\mu\nu}\right) = \frac{1}{\alpha}\partial_t K_{\mu\nu} - \frac{1}{\alpha}\mathcal{L}_{\boldsymbol{\beta}}K_{\mu\nu}\,, \tag{F.91}$$

where we have used that the Lie derivative along a coordinate vector equals the partial derivative with respect to this coordinate. The corresponding equation for $\gamma_{\alpha\beta}$ is derived in exactly the same way. □

Since the shift vector is spatial, we can compute the Lie derivatives along $\boldsymbol{\beta}$ using the standard definition in three dimensions,

$$\begin{aligned}
\mathcal{L}_{\boldsymbol{\beta}}\gamma_{ij} &= \beta^m\partial_m\gamma_{ij} + \gamma_{mj}\partial_i\beta^m + \gamma_{im}\partial_j\beta^m \;=\; \beta^m\partial_m\gamma_{ij} + 2\gamma_{m(i}\partial_{j)}\beta^m\,, && \text{(F.92)} \\
\mathcal{L}_{\boldsymbol{\beta}}K_{ij} &= \beta^m\partial_m K_{ij} + K_{mj}\partial_i\beta^m + K_{im}\partial_j\beta^m \;=\; \beta^m\partial_m K_{ij} + 2K_{m(i}\partial_{j)}\beta^m\,. && \text{(F.93)}
\end{aligned}$$

Likewise, we can now compute the three-dimensional Christoffel symbols and Riemann tensor from their standard expressions analogous to Eq. (A.1),

$$\begin{aligned}
\Gamma^i_{jk} &= \frac{1}{2}\gamma^{im}\left(\partial_j\gamma_{km} + \partial_k\gamma_{mj} - \partial_m\gamma_{jk}\right)\,, && \text{(F.94)} \\
\mathcal{R}^j{}_{kmn} &= \partial_m\Gamma^j_{kn} - \partial_n\Gamma^j_{km} + \Gamma^l_{kn}\Gamma^j_{lm} - \Gamma^l_{km}\Gamma^j_{ln}\,. && \text{(F.95)}
\end{aligned}$$

Finally, we replace Greek spacetime with Latin spatial indices in Eqs. (F.71)-(F.74).

Proposition: The ADM or 3+1 formulation of the Einstein equations is

$$\mathcal{H} \;:=\; \mathcal{R} + K^2 - K_{mn}K^{mn} - 2\Lambda - 16\pi\rho = 0\,, \tag{F.96}$$

$$\mathcal{M}_i \;:=\; D_i K - D_m K_i{}^m + 8\pi j_i = 0\,, \tag{F.97}$$

$$\partial_t \gamma_{ij} = \beta^m \partial_m \gamma_{ij} + 2\gamma_{m(i}\partial_{j)}\beta^m - 2\alpha K_{ij}\,, \tag{F.98}$$

$$\begin{aligned}\partial_t K_{ij} = {}& \beta^m \partial_m K_{ij} + 2K_{m(i}\partial_{j)}\beta^m - D_i D_j \alpha + \alpha\left[\mathcal{R}_{ij} + KK_{ij} - 2K_{im}K^m{}_j\right] \\ & -\alpha\Lambda\gamma_{ij} - 8\pi\alpha\left[S_{ij} - \frac{1}{2}\gamma_{ij}(S-\rho)\right]\,.\end{aligned} \tag{F.99}$$

Note that these equations fully confirm the structure of the Einstein equations that we have uncovered in Sec. D. We have four equations that contain no time derivatives, the Hamiltonian and momentum constraints (F.96), (F.97), and 6 evolution equations written as a first-order system in Eqs. (F.98) and (F.99). As we have already shown on Page 44, the constraints are preserved under the evolution equations. Furthermore, the Einstein equations do not determine the four gauge variables α and β^i; these can be freely chosen and represent the coordinate freedom of general relativity. Finally, we can count the degrees of freedom: We start with 10 components of the spacetime metric $g_{\alpha\beta}$. Four of these, the lapse and shift, can be chosen freely leaving us with the 6 variables γ_{ij}. The constraints impose 4 conditions on these 6 functions, leaving 2 second-order in time degrees of freedom as expected.

For completeness, we list here without proof the 3+1 evolution equations for the matter variables which are obtained from projecting the conservation of energy and momentum, $\nabla_\mu T^{\alpha\mu} = 0$ onto time and space.

Proposition: The energy density ρ and momentum density j_i obey the 3+1 evolution equations

$$\partial_t \rho = \beta^m \partial_m \rho - 2j^m D_m \alpha + \alpha\left(\rho K + S^{mn}K_{mn} - D_m j^m\right)\,, \tag{F.100}$$

$$\partial_t j_i = \beta^m \partial_m j_i + j_m \partial_i \beta^m - \rho D_i \alpha - S^m{}_i D_m \alpha + \alpha\left(j_i K - D_m S^m{}_i\right)\,. \tag{F.101}$$

Note that we do not have an evolution equation for the stress tensor S_{ij}. This is expected, since the evolution of the matter will depend on the type of matter under consideration. It is therefore necessary to specify additional information about the matter; this often comes in the form of an equation of state that prescribes the pressure as a function other matter variables such as the energy density. This additional information then determines the stress tensor in terms of the evolved variables ρ and j_i. For a discussion of perfect fluids, for example, see Sec. 5.3 in Gourgoulhon's review [24].

With the ADM equations, we have now at our disposal a formulation of the Einstein equations as a constrained initial value problem. Unfortunately, this formulation is of limited practical value in numerical implementations. The reason is that the resulting equations are in general not mathematically well posed. Well-posedness can, however, be achieved by modifying the ADM equations using a conformal decomposition. How the problems arise and what we can do to overcome them is the next stage in our odyssey.

G Well-posedness, strong hyperbolicity and BSSNOK

G.1 The concept of well-posedness

The study of the well-posedness of the different formulations of the Einstein equations is still an active area of research and extends well beyond the scope of these lectures. In this section, we will therefore pursue the more humble goal of indicating for the case of a simple example, how ill-posedness can arise in partial differential equations and how this property can be studied analytically. In our discussion we follow the PhD thesis of Giuseppe Papallo [25] where readers can also find a much more detailed discussion of this subject.

Def. : An initial value (aka Cauchy) problem is *well-posed* if a solution exists, is unique and depends continuously on the initial data in the sense of a norm $||f(t,.)||$ commonly taken to be the spatial $L2$ norm of a function $f(t,x^i)$ at fixed time t. If these conditions are not met, the initial-value problem is *ill-posed*.

Examples

(1) The potentially problematic issue of well/ill posedness is best illustrated by regarding the two-dimensional Laplace equation as an initial-value problem; in fact it was this specific study that led Hadamard to the above definition of well-posedness. In order to emphasize our viewpoint of a Cauchy problem, we denote the coordinates by (t,x) rather than the more common (x,y); of course this change of variables does not alter the equation and its properties in any way. We are thus looking for solutions $\phi(t,x)$ of the PDE

$$\Delta\phi(t,x) = \partial_t^2\phi + \partial_x^2\phi = 0\,, \tag{G.1}$$

with initial data

$$\phi(0,x) = f(x)\,, \qquad \partial_t\phi(0,x) = g(x)\,.$$

For the specific choice of initial data

$$f_n(x) = 0\,, \qquad g_n(x) = e^{-\sqrt{n}}\sin(nx)\,,$$

the solution is given by

$$\phi_n(t,x) = \frac{e^{-\sqrt{n}}}{n}\sinh(nt)\,\sin(nx)\,, \tag{G.2}$$

as can be readily confirmed by inserting into Eq. (G.1). Taking the limit $n\to\infty$, the initial data converge to zero,

$$\lim_{n\to\infty} f_n(x) =: f_\infty = 0\,, \qquad \lim_{n\to\infty} g_n(x) =: g_\infty = 0\,, \tag{G.3}$$

whereas the solution (G.2) blows up exponentially for any non-zero value of t. If we denote by ϕ_∞ the time evolution of the initial data f_∞, g_∞, we clearly have

$$\lim_{n\to\infty}||\phi_n - \phi_\infty|| = \infty \quad \text{whereas} \quad \lim_{n\to\infty}||f_n - f_\infty|| = 0\,,\ \ \lim_{n\to\infty}||g_n - g_\infty|| = 0\,, \tag{G.4}$$

and the solution at finite t does not depend continuously on the initial data.

(2) One can show that this problem does not arise for the wave equation where we merely change the sign in front of the second time derivative,

$$\Box\phi(t,x) = -\partial_t^2\phi + \partial_x^2 = 0\,, \tag{G.5}$$

with initial data

$$\phi(0,x) = f(x)\,, \qquad \partial_t\phi(0,x) = g(x)\,.$$

(3) The vacuum Maxwell equations for a magnetic field $\boldsymbol{B}(t,\boldsymbol{x})$ and an electric field $\boldsymbol{E}(t,\boldsymbol{x})$ can be formulated as a system of linear wave equations in three dimensions,

$$\Box\boldsymbol{B}(t,\boldsymbol{x}) = 0\,, \qquad \Box\boldsymbol{E}(t,\boldsymbol{x}) = 0\,, \tag{G.6}$$

with initial data $\boldsymbol{B}(0,\boldsymbol{x})$, $\boldsymbol{E}(0,\boldsymbol{x})$, $\partial_t\boldsymbol{B}(0,\boldsymbol{x})$, $\partial_t\boldsymbol{E}(0,\boldsymbol{x})$ subject to the constraints

$$\nabla\cdot\boldsymbol{E}(t,\boldsymbol{x}) = 0\,, \qquad \nabla\cdot\boldsymbol{B}(t,\boldsymbol{x}) = 0\,. \tag{G.7}$$

These equations can also be shown to be well posed. Note the similarity to the structure of the Einstein equations with evolution and constraint equations. In fact, the Maxwell constraints are preserved under time evolution provided they are satisfied initially, in complete analogy to what we have seen for the Hamiltonian and momentum constraints in GR.

G.2 Well-posedness of first-order systems

The well-posedness of PDE systems is most conveniently studied for first-order systems. In fact, the corresponding study of second- or higher-order PDE systems is commonly performed by reducing these systems to first-order through the introduction of auxiliary variables; readers interested in more details can find these in Sec. 2.3 of Papallo's thesis [25].

As is often the case with studies of PDEs, the concept of well-posedness is rigorously formulated for linear systems with constant coefficients. The results are then generalized to linear systems in the sense of local well-posedness, considering a neighbourhood of some point in the domain where the coefficient matrices do not significantly vary. The well-posedness of non-linear PDEs is then studied by linearizing around some background and demonstrating that local well-posedness is obtained for arbitrary backgrounds. In practice, one often considers only a certain set of common backgrounds like the Schwarzschild solution, Minkowski or Friedmann-Lemître-Robertson-Walker, thus obtaining candidate systems of well-posed character whose well-posedness can be tested in experimental simulations. The beneficial features of the Baumgarte-Shapiro-Shibata-Nakamura-Oohara-Kojima (BSSNOK)[10] [26, 27, 28] formulation – still the most popular formulation in numerical relativity – have actually been identified empirically before its potential[11] well-posedness was demonstrated analytically.

[10] In the literature, this formulation is often abbreviated to BSSN.

[11] We add the qualifier "potential" here, since the well-posedness of a given formulation of GR depends on the gauge conditions used.

Throughout this section, we consider PDEs on a $d+1$ dimensional domain $\Omega \subset \mathbb{R}^{d+1}$ with coordinates (t, x_i) where $i = 1, \ldots, d$. The picture we have in mind here is a domain with d spatial dimensions and one time direction along which data is evolved. We consider vector valued functions $\boldsymbol{u} : \Omega \subset \mathbb{R}^{d+1} \to \mathbb{R}^N$ satisfying the PDE system

$$\mathbf{A}\partial_t \boldsymbol{u} + \mathbf{P}^i \partial_i \boldsymbol{u} + \mathbf{C}\boldsymbol{u} = 0\,, \tag{G.8}$$

where $\mathbf{A}$, each $\mathbf{P}^i$ and $\mathbf{C}$ are real $N \times N$ matrices and $\mathbf{A}$ is invertible.

As mentioned above, we first consider the case where $\mathbf{A}$, $\mathbf{P}^i$ and $\mathbf{C}$ all have constant components independent of (t, x_i). Defining the Fourier transform of a function $f(x_i)$ in d spatial dimensions and its inverse by

$$\begin{aligned} \tilde{f}(k_i) &= \mathcal{F}[f](k_i) &= \frac{1}{\sqrt{2\pi}^d}\int f(x_i) e^{-\mathrm{i}k_m x_m} \mathrm{d}^d x\,, \\ f(x_i) &= \mathcal{F}^{-1}[\tilde{f}](x_i) &= \frac{1}{\sqrt{2\pi}^d}\int \tilde{f}(k_i) e^{\mathrm{i}k_m x_m} \mathrm{d}^d x\,, \end{aligned} \tag{G.9}$$

where we sum over repeated indices, we can compute the Fourier transform of a spatial derivative using partial integration,

$$\mathcal{F}[\partial_i f](k_i) = \frac{1}{\sqrt{2\pi}^d}\int \partial_i f\, e^{-\mathrm{i}k_m x_m} \mathrm{d}^d x = -\frac{1}{\sqrt{2\pi}^d}\int f\, \partial_i \left(e^{-\mathrm{i}k_m x_m}\right) \mathrm{d}^d x = \mathrm{i}k_i \tilde{f}(k_i)\,. \tag{G.10}$$

Here the boundary term drops out because square-integrable functions vanish at infinity. Fourier transforming the entire PDE (G.8) gives us,

$$\begin{aligned} & \mathbf{A}\partial_t \tilde{\boldsymbol{u}} + \mathbf{P}^m \mathrm{i}k_m \tilde{\boldsymbol{u}} + \mathbf{C}\tilde{\boldsymbol{u}} = 0 \\ \Rightarrow \quad & \partial_t \tilde{\boldsymbol{u}} + \mathbf{A}^{-1}\left(\mathrm{i}\mathbf{P}^m k_m + \mathbf{C}\right)\tilde{\boldsymbol{u}} = \partial_t \tilde{\boldsymbol{u}} - \mathrm{i}\Big[\underbrace{\mathbf{A}^{-1}\left(-\mathbf{P}^m k_m + \mathrm{i}\mathbf{C}\right)}_{=:\mathbf{M}(k_m)}\Big]\tilde{\boldsymbol{u}}\,. \end{aligned} \tag{G.11}$$

The solution to the transformed PDE (G.11) with initial data $\tilde{\boldsymbol{u}}(0, k_i)$ is then given by

$$\tilde{\boldsymbol{u}}(t, k_i) = e^{\mathrm{i}\mathbf{M}t}\tilde{\boldsymbol{u}}(0, k_i)\,, \quad \text{with} \quad \mathbf{M} = \mathbf{A}^{-1}(-\mathbf{P}^m k_k + \mathrm{i}\mathbf{C})\,, \tag{G.12}$$

and the solution to the original PDE (G.8) is reconstructed from the inverse Fourier transform

$$\boldsymbol{u}(t, x_i) = \frac{1}{\sqrt{2\pi}^d}\int e^{\mathrm{i}\mathbf{M}t}\tilde{\boldsymbol{u}}(0, k_i) e^{\mathrm{i}k_m x_m} \mathrm{d}^d k\,. \tag{G.13}$$

For $t = 0$, the integral on the right-hand side converges since we have by assumption regular initial data $\boldsymbol{u}(0, x_i)$. But we have no guarantee that the integral converges and, hence, yields a regular solution $\boldsymbol{u}(t, x_i)$ for $t > 0$. To proceed with our quest to understand well-posedness, we need to investigate under which conditions the integral in Eq. (G.13) converges.

Proposition: If there exists a regular function f such that

$$\left|\left|e^{\mathrm{i}\mathbf{M}t}\right|\right| \leq f(t) \quad \text{with} \quad \mathbf{M} = \mathbf{A}^{-1}(-\mathbf{P}^m k_k + \mathrm{i}\mathbf{C})\,, \tag{G.14}$$

then the right-hand side of Eq. (G.13) converges and the PDE (G.8),

$$\mathbf{A}\partial_t \boldsymbol{u} + \mathbf{P}^m \partial_m \boldsymbol{u} + \mathbf{C}\boldsymbol{u} = 0\,,$$

with constant matrices is well posed.

Proof. If $||e^{\mathrm{i}\mathbf{M}t}|| < f(t)$, taking the norm of Eq. (G.12) gives us

$$||\tilde{\boldsymbol{u}}||(t) = \left|\left|e^{\mathrm{i}\mathbf{M}t}\right|\right| \times ||\tilde{\boldsymbol{u}}||(0) \leq f(t)||\tilde{\boldsymbol{u}}||(0)\,. \tag{G.15}$$

By Parseval's theorem (also know as Plancherel's identity), this implies

$$||\boldsymbol{u}||(t) \leq f(t)||\boldsymbol{u}||(0)\,, \tag{G.16}$$

so the inverse Fourier transform (G.13) with finite norm exists.

For the well-posedness of the PDE (G.8), we consider two solutions $\boldsymbol{u}_1$, $\boldsymbol{u}_2$ corresponding to initial data $\boldsymbol{u}_1(0,x_i)$ and $\boldsymbol{u}_2(0,x_i)$. By linearity of the PDE, the difference is also a solution, so that

$$||\boldsymbol{u}_1 - \boldsymbol{u}_2||(t) \leq f(t)||\boldsymbol{u}_1 - \boldsymbol{u}_2||(0)\,. \tag{G.17}$$

The solution of the PDE therefore depends continuously on the initial data. We also see that the solution for given initial data is unique since $\boldsymbol{u}_1(0,x_i) = \boldsymbol{u}_2(0,x_i)$ implies $||\boldsymbol{u}_1 - \boldsymbol{u}_2||(0) = 0$ and therefore $\boldsymbol{u}_1(t,x_i) - \boldsymbol{u}_2(t,x_i) \leq f(t) \times 0 = 0$, so $\boldsymbol{u}_1 = \boldsymbol{u}_2$. □

Our next step is to obtain a criterion that ensures Eq. (G.14) holds. We start with a necessary condition.

The PDE

$$\mathbf{A}\partial_t \boldsymbol{u} + \mathbf{P}^m \partial_m \boldsymbol{u} + \mathbf{C}\boldsymbol{u} = 0\,,$$

with constant matrices $\mathbf{A}$, $\mathbf{P}^m$ and $\mathbf{C}$ is *weakly hyperbolic* if for any wave vector $\hat{k}_i$ with unit norm, $|\hat{k}| = 1$, all Eigenvalues of

$$\mathbf{Q}(\hat{k}_i) := -\mathbf{A}^{-1}\mathbf{P}^m \hat{k}_m\,, \tag{G.18}$$

are real.

Proposition: Weak hyperbolicity of the PDE (G.8) is a necessary condition for $||e^{\mathrm{i}\mathbf{M}t}|| \leq f(t)$ to hold for a regular function $f(t)$.

Proof. Define

$$\hat{t} := |k|\, t\,, \qquad \hat{k}_i := \frac{k_i}{|k|}\,, \tag{G.19}$$

so that Eq. (G.14) becomes

$$\left|\left|e^{\mathrm{i}\mathbf{M}\hat{t}/|k|}\right|\right| = \left|\left|e^{\mathrm{i}\left[\mathbf{A}^{-1}(-\mathbf{P}^m k_m + \mathrm{i}\mathbf{C})\right]\hat{t}/|k|}\right|\right| = \left|\left|e^{\mathrm{i}\left[\mathbf{A}^{-1}(-\mathbf{P}^m \hat{k}_m + \mathrm{i}\mathbf{C}/|k|)\right]\hat{t}}\right|\right| \leq f\left(\tfrac{\hat{t}}{|k|}\right) \tag{G.20}$$

Note that our rescaling of k_i and t stresses the dominance of short-wavelength modes: Modes with large $|k|$ effect substantial evolution in terms of the rescaled time $\hat{t}$ even for very short steps in physical time t. This is not surprising if we consider the original PDE written as

$$\partial_t \boldsymbol{u} = -\mathbf{A}^{-1}\mathbf{P}^m \partial_m \boldsymbol{u} - \mathbf{A}^{-1}\mathbf{C}\boldsymbol{u}\,.$$

Modes with very short wavelength have large gradients $\partial_m \boldsymbol{u}$ which rapidly drive the evolution of $\boldsymbol{u}$ in time, completely dominating over the $\mathbf{C}\boldsymbol{u}$ term. Here lies the reason why the structure of PDEs is dominated by its principal part, i.e. its highest derivative terms: Short wavelength modes determine the convergence of the inverse Fourier transform and predominantly act through the highest derivative terms in the PDE. But let us continue with our proof.

Taking the limit $|k| \to \infty$ at constant $\hat{t}$, Eq. (G.20) becomes

$$\left|\left|e^{\mathrm{i}\mathbf{Q}(\hat{k}_i)\hat{t}}\right|\right| \leq f(0) \qquad \text{with} \qquad \mathbf{Q}(\hat{k}_i) = -\mathbf{A}^{-1}\mathbf{P}^m \hat{k}_m\,. \tag{G.21}$$

Note that this equation must hold for arbitrarily large $\hat{t}$ since for short-wavelength modes with $|k| \to \infty$, even the smallest advance in physical time t implies $\hat{t} \to \infty$.

Next we consider an Eigenvector $\boldsymbol{V}$ of $\mathbf{Q}$ with Eigenvalue $\lambda = \lambda_1 + \mathrm{i}\lambda_2$, so that

$$e^{\mathrm{i}\mathbf{Q}\hat{t}}\boldsymbol{V} = e^{\mathrm{i}\lambda_1 \hat{t}} e^{-\lambda_2 \hat{t}} \boldsymbol{V}\,. \tag{G.22}$$

Equation (G.21) can only be satisfied for arbitrarily large $\hat{t}$ if $\lambda_2 \geq 0$. But $\mathbf{Q}$ is a real matrix, so if λ is an Eigenvalue, then its complex conjugate $\bar{\lambda} = \lambda_1 - \mathrm{i}\lambda_2$ is also an Eigenvalue. Equation (G.21) can therefore only be satisfied if $\lambda_2 = 0$, i.e. if all Eigenvalues of $\mathbf{Q}$ are real. □

The ADM equations discussed in Sec. F can be shown to be weakly hyperbolic; see e.g. [29]. Unfortunately, weak hyperbolicity is not sufficient for well-posedness. The reason is that off-diagonal terms that appear in the Jordan-normal form of the matrix $\mathbf{Q}$, while avoiding exponential violation of Eq. (G.21), still lead to polynomial violation of this bound.

Lemma : Let

$$\mathbf{J}_2 = \begin{pmatrix} \lambda & 1 \\ 0 & \lambda \end{pmatrix}\,, \qquad \text{with} \qquad \lambda \in \mathbb{C}\,. \tag{G.23}$$

Then

$$e^{\mathrm{i}\mathbf{J}_2 \hat{t}} = e^{\mathrm{i}\lambda\hat{t}} \begin{pmatrix} 1 & \mathrm{i}\hat{t} \\ 0 & 1 \end{pmatrix}\,. \tag{G.24}$$

Proof.

$$e^{\mathrm{i}\mathbf{J}_2\hat{t}} = \mathbb{1} + (\mathrm{i}\mathbf{J}_2\hat{t}) + \frac{1}{2!}(\mathrm{i}\mathbf{J}_2\hat{t})^2 + \frac{1}{3!}(\mathrm{i}\mathbf{J}_2\hat{t})^3 + \ldots \tag{G.25}$$

The pattern of the powers of $\mathbf{J}_2$ is quickly understood by computing

$$\begin{aligned}
\begin{pmatrix} \lambda & 1 \\ 0 & \lambda \end{pmatrix}^2 &= \begin{pmatrix} \lambda^2 & 2\lambda \\ 0 & \lambda^2 \end{pmatrix}, \\
\begin{pmatrix} \lambda & 1 \\ 0 & \lambda \end{pmatrix}^3 &= \begin{pmatrix} \lambda^3 & 3\lambda^2 \\ 0 & \lambda^3 \end{pmatrix}, \\
\begin{pmatrix} \lambda & 1 \\ 0 & \lambda \end{pmatrix}^n &= \begin{pmatrix} \lambda^n & n\lambda^{n-1} \\ 0 & \lambda^n \end{pmatrix},
\end{aligned} \tag{G.26}$$

so that

$$e^{\mathrm{i}\mathbf{J}_2\hat{t}} = \begin{pmatrix} e^{\mathrm{i}\lambda\hat{t}} & x \\ 0 & e^{\mathrm{i}\lambda\hat{t}} \end{pmatrix}, \tag{G.27}$$

with

$$\begin{aligned}
x &= 0 + \mathrm{i}\hat{t} + \frac{1}{2!}(\mathrm{i}\hat{t})^2 2\lambda + \frac{1}{3!}(\mathrm{i}\hat{t})^3 3\lambda^2 + \ldots \\
&= \mathrm{i}\hat{t}\left[1 + \mathrm{i}\lambda\hat{t} + \frac{1}{2!}(\mathrm{i}\lambda\hat{t})^2 + \ldots\right] = \mathrm{i}\hat{t}e^{\mathrm{i}\lambda\hat{t}}.
\end{aligned} \tag{G.28}$$

□

Returning to Eq. (G.21), we see that $\left|\left|\exp\left[\mathrm{i}\mathbf{Q}(\hat{k}_i)\hat{t}\right]\right|\right|$ cannot be bound by a constant $f(0)$ if it contains a Jordan block of the form (G.23). One can likewise show that larger Jordan blocks of type $n \times n$ also give rise to terms $\propto (\hat{t})^p$ in $e^{\mathrm{i}\mathbf{Q}\hat{t}}$ for some $1 \leq p \leq n$ and therefore spoil the condition (G.21). The only way to avoid these polynomial terms is a diagonalizable matrix $\mathbf{Q}$.

Def. : The PDE $\mathbf{A}\partial_t\boldsymbol{u} + \mathbf{P}^m\partial_m\boldsymbol{u} + \mathbf{C}\boldsymbol{u} = 0$ with constant coefficient matrices is *strongly hyperbolic* if for all wave vectors $\hat{k}_i$ with unit norm, $\mathbf{Q} = -\mathbf{A}^{-1}\mathbf{P}^m\hat{k}_m$ has only real Eigenvalues and is diagonalizable, i.e. there exists a matrix $\mathbf{S}(\hat{k}_i)$ such that $\mathbf{Q} = \mathbf{S}\mathbf{D}\mathbf{S}^{-1}$ where $\mathbf{D}(\hat{k}_i)$ is diagonal. If the matrix $\mathbf{S}$ does not depend on $\hat{k}_i$, the PDE is *symmetric hyperbolic*.

So far, our investigation is restricted to linear PDEs with constant coefficients. As indicated above, the conditions for well-posedness are extended to linear PDEs by considering the local well-posedness in a neighbourhood of some point $(t_0, \boldsymbol{x}_0)$ where the coefficient matrices $\mathbf{A}$, $\mathbf{P}^m$ and $\mathbf{C}$ are regarded as frozen at their values at the point $(t_0, \boldsymbol{x}_0)$. The justification for this generalization is that well-posedness is a feature of short-wavelength modes, so that it is sufficient to consider small neighbourhoods. This motivates the following definition.

Def. : The linear PDE $\mathbf{A}\partial_t \boldsymbol{u} + \mathbf{P}^m \partial_m \boldsymbol{u} + \mathbf{C}\boldsymbol{u} = 0$ is *weakly hyperbolic* if for all (t, x_i) and $\hat{k}_i$ with $|\hat{k}| = 1$, all Eigenvalues of $\mathbf{Q}(t, x_i, \hat{k}_i) = -\mathbf{A}(t, x_i)^{-1}\mathbf{P}^m(t, x_i)k_m$ are real. The PDE is strongly hyperbolic if $\mathbf{Q}$ is furthermore diagonalizable for all (t, x_i) and $\hat{k}_i$. The The PDE is *symmetric hyperbolic* if it is strongly hyperbolic and the symmetrizer $\mathbf{S}$ is independent of $\hat{k}_i$.

Readers may have noticed that our chain of conditions for well-posedness is a mixture of sufficient and necessary conditions. Our recipe for analyzing the well-posedness of a given PDE system is therefore not entirely rigorous. Violating strong hyperbolicity does not imply ill-posedness with 100 % certainty and strong hyperbolicity does not guarantee well-posedness. The well-posedness of non-linear PDEs is furthermore limited to studying the linearized equations around generic backgrounds. The development of stable numerical codes therefore inevitably involves empirical tests. The experience accumulated by the numerical relativity community over about five decades has established with high reliability that weakly hyperbolic formulations like the ADM equations are almost guaranteed to result in numerical instability on short timescales compared to the relevant timescales of the physical systems under consideration. For example, all long-term stable evolutions of black-hole binaries employ strongly or symmetric hyperbolic formulations. It should be noted, however, that even in that case, suitable gauge conditions and stable numerical algorithms are required to obtain reliable simulations.

G.3 The BSSNOK formulation

The ADM formulation of the Einstein equations was used for most 3+1 simulations of the Einstein equations well into the 1990s, despite the ubiquitous instabilities encountered in these simulations. The realization that these problems might be a feature of the ADM equations themselves (rather than the numerical algorithms employed for their evolution) gradually became accepted by the community during the 1990s. As we have already noted above, however, this realization came about through a mixture of empirical observation and suspicion; the weakly hyperbolic character of the ADM equations was not understood until the early 2000s. The vast improvements achieved in numerical simulations using the BSSNOK formulation (e.g. [27, 30, 31]) played a key role in this realization. Following this empirical success, the capacity of the BSSNOK system to result in strongly hyperbolic equations has been studied intensively; see e.g. [32, 33].

We also note that the search for well-posed formulations is by no means restricted to the BSSNOK system. Various other formulations have been studied and implemented in numerical codes including the Kidder-Scheel-Teukolsky (KST) system [34], the Nagy-Ortiz-Reula (NOR) formulation [35], the generalized harmonic gauge (GHG) formulation [36, 37, 38] and the conformal $Z4$ formulation [39, 40, 41]. Indeed, the very first BH binary inspiral and merger simulations by Pretorius [7] was obtained with the GHG formulation, followed and confirmed about half a year later by the so-called *moving puncture* breakthroughs of the Brownsville and Goddard groups using BSSNOK [8, 9]. In recent years, the conformal $Z4$ formalism has become a particularly popular alternative to the BSSNOK formulation. We could easily arrange an entire Part III course on any of these formulations. Here, we have to focus our energy and opt for a more detailed discussion of the BSSNOK system for two main reasons. (i) Its close relation to the ADM equations makes it comparatively simple to derive and (ii) it suitably illustrates the type of modifications that facilitate improvements over the ADM system. We start our derivation by recalling some useful relations.

Proposition: Let $g_{\alpha\beta}$ be the metric, with arbitrary signature, of an n dimensional manifold with inverse $g^{\alpha\beta}$. Then the determinant $g \coloneqq \det g_{\alpha\beta}$ satisfies

$$\frac{\partial g}{\partial g_{\alpha\beta}} = g\, g^{\alpha\beta}\,, \qquad \frac{\partial g}{\partial g^{\alpha\beta}} = -g\, g_{\alpha\beta}\,. \tag{G.29}$$

It follows that

$$\partial_\alpha g = \frac{\partial g}{\partial g_{\mu\nu}} \partial_\alpha g_{\mu\nu} = g\, g^{\mu\nu} \partial_\alpha g_{\mu\nu} = -g\, g_{\mu\nu} \partial_\alpha g^{\mu\nu} = 2g \Gamma^\mu_{\mu\alpha}\,. \tag{G.30}$$

Proof. We recall that the inverse of a matrix a_{ij} is given by first constructing the co-factor matrix C_{ij}, crossing out row i and column j in a_{ij}, computing the determinant of the remnant and then multiplying with $(-1)^{i+j}$. The adjunct C_{ji} divided by $\det a_{ij}$ gives us the inverse matrix $(a^{-1})_{ij}$. On the other hand, we can compute $a \coloneqq \det a_{ij}$ by expanding in the ith row using the corresponding co-factor matrices,

$$a = \det a_{ij} = \sum_j a_{ij} C_{ij} \quad \Rightarrow \quad \frac{\partial a}{\partial a_{ik}} = C_{ik} \overset{!}{=} (a^{-1})_{ki}\, a\,. \tag{G.31}$$

Applying this relation to the metric $g_{\alpha\beta}$ and bearing in mind its symmetry, we obtain

$$\frac{\partial g}{\partial g_{\alpha\beta}} = g\, g^{\beta\alpha} = g\, g^{\alpha\beta}\,, \tag{G.32}$$

which is the first equation above. For the second equation we exchange metric and inverse metric which gives us

$$\frac{\partial g^{-1}}{\partial g^{\alpha\beta}} = -\frac{1}{g^2} \frac{\partial g}{\partial g^{\alpha\beta}} \overset{!}{=} g^{-1}\, g_{\alpha\beta} \qquad \Rightarrow \qquad \frac{\partial g}{\partial g^{\alpha\beta}} = -g\, g_{\alpha\beta}\,. \tag{G.33}$$

Therefore,

$$\partial_\alpha g = \frac{\partial g}{\partial g_{\mu\nu}} \partial_\alpha g_{\mu\nu} = g\, g^{\mu\nu} \partial_\alpha g_{\mu\nu} = -g\, g_{\mu\nu} \partial_\alpha g^{\mu\nu}\,, \tag{G.34}$$

which also follows from $g^{\mu\nu} g_{\mu\nu} = 4 = \text{const}$. The final equality follows from the vanishing of the covariant derivative of the metric,

$$\nabla_\alpha g_{\mu\nu} = \partial_\alpha g_{\mu\nu} - \Gamma^\rho_{\mu\alpha} g_{\rho\nu} - \Gamma^\rho_{\nu\alpha} g_{\mu\rho} = 0$$

$$\Rightarrow \quad \partial_\alpha g = g\, g^{\mu\nu} \left(\Gamma^\rho_{\mu\alpha} g_{\rho\nu} + \Gamma^\rho_{\nu\alpha} g_{\mu\rho} \right) = 2g \Gamma^\mu_{\mu\alpha}\,. \tag{G.35}$$

Note that theses results apply in analogy to the spatial metric γ_{ij}. □

Def. : The BSSNOK variables are defined in terms of the ADM variables by[12]

$$
\begin{aligned}
\chi &= \gamma^{-1/3}\,, & K &= \gamma^{mn}K_{mn}, \\
\tilde{\gamma}_{ij} &= \chi\gamma_{ij} & \Leftrightarrow\quad \tilde{\gamma}^{ij} &= \frac{1}{\chi}\gamma^{ij}, \\
\tilde{A}_{ij} &= \chi\left(K_{ij} - \tfrac{1}{3}\gamma_{ij}K\right) & \Leftrightarrow\quad K_{ij} &= \frac{1}{\chi}\left(\tilde{A}_{ij} + \frac{1}{3}\tilde{\gamma}_{ij}K\right)\,, \\
\tilde{\Gamma}^i &= \tilde{\gamma}^{mn}\tilde{\Gamma}^i_{mn}\,,
\end{aligned}
\tag{G.36}
$$

Note that these definitions imply two algebraic and one differential constraints,

$$
\tilde{\gamma} = 1\,, \qquad \tilde{\gamma}^{mn}\tilde{A}_{mn} = 0\,, \qquad \mathcal{G}^i := \tilde{\Gamma}^i - \tilde{\gamma}^{mn}\tilde{\Gamma}^i_{mn} = 0\,. \tag{G.37}
$$

In words, we apply a conformal decomposition to the spatial metric such that the conformal metric has unit determinant, we split the extrinsic curvature into trace and traceless part and apply the same conformal transformation to the latter. Finally, we promote the contracted Christoffel symbols to the status of free variables. Two key benefits arise from this rearrangement of the degrees of freedom. First, we have isolated much of the spacetime curvature inside the two variables χ and K rather than all twelve components of the metric and extrinsic curvature. Second, one can show that introducing the $\tilde{\Gamma}^i$ as evolution variables eliminates most second derivatives from the Ricci tensor, leaving only the spatial part of the wave operator, $\tilde{\gamma}^{mn}\partial_m\partial_n\tilde{\gamma}_{ij}$; see Eq. (G.76) below. Given the well-posedness of the wave equation, this is regarded a key ingredient of the BSSNOK formulation. We start our derivation of the BSSNOK equations with some auxiliary relations.

Lemma : The Christoffel symbols associated with the physical metric γ_{ij} and the conformal metric $\tilde{\gamma}_{ij}$ are related by

$$
\Gamma^i_{jk} = \tilde{\Gamma}^i_{jk} - \frac{1}{2\chi}\left(\delta^i{}_k\partial_j\chi + \delta^i{}_j\partial_k\chi - \tilde{\gamma}_{jk}\tilde{\gamma}^{im}\partial_m\chi\right)\,. \tag{G.38}
$$

Proof. Using $\tilde{\gamma}_{ij} = \chi\gamma_{ij}$ and product rule, we get

$$
\begin{aligned}
\Gamma^i_{jk} &= \frac{1}{2}\gamma^{im}\left(\partial_j\gamma_{km} + \partial_k\gamma_{mj} - \partial_m\gamma_{jk}\right) \\
&= \frac{1}{2}\tilde{\gamma}^{im}\left(\partial_j\tilde{\gamma}_{km} + \partial_k\tilde{\gamma}_{mj} - \partial_m\tilde{\gamma}_{jk}\right) + \frac{1}{2}\chi\tilde{\gamma}^{im}\left(\tilde{\gamma}_{km}\partial_j\frac{1}{\chi} + \tilde{\gamma}_{mj}\partial_k\frac{1}{\chi} - \tilde{\gamma}_{jk}\partial_m\frac{1}{\chi}\right)
\end{aligned}
$$

[12] In place of the variable χ, some numerical relativity codes have used with comparable success the alternative variables $\phi := -(\ln\chi)/4$ or $W := \sqrt{\chi}$.

$$= \tilde{\Gamma}^i_{jk} - \frac{1}{2\chi}\left(\delta^i{}_k\partial_j\chi + \delta^i{}_j\partial_k\chi - \tilde{\gamma}_{jk}\tilde{\gamma}^{im}\partial_m\chi\right) . \tag{G.39}$$

□

Lemma : A metric γ_{ij} and its inverse are related by

$$\partial_i\gamma^{jk} = -\gamma^{jm}\gamma^{kn}\partial_i\gamma_{mn} \,, \qquad \partial_i\gamma_{jk} = -\gamma_{jm}\gamma_{kn}\partial_i\gamma^{mn}$$

$$\Rightarrow \quad \partial_k\gamma^{jk} = -\gamma^{jm}\gamma^{kn}\partial_k\gamma_{mn} \,. \tag{G.40}$$

These relations hold in complete analogy for the spacetime metric $g_{\alpha\beta}$ and the conformal spatial metric $\tilde{\gamma}_{ij}$. For the conformal metric, $\tilde{\gamma} = 1$ implies

$$\tilde{\Gamma}^i = \tilde{\gamma}^{mn}\tilde{\gamma}^{il}\partial_m\tilde{\gamma}_{nl} = -\,\partial_m\tilde{\gamma}^{mi} \,, \tag{G.41}$$

$$\tilde{\Gamma}^m_{im} = \frac{1}{2}\tilde{\gamma}^{mn}\partial_i\tilde{\gamma}_{mn} = 0 \,. \tag{G.42}$$

Proof.

$$0 = \partial_i\delta^j{}_k = \partial_i(\gamma^{jm}\gamma_{mk}) = \gamma^{jm}\partial_i\gamma_{mk} + \gamma_{mk}\partial_i\gamma^{jm} \qquad \Big| \quad \times\gamma^{kl} \quad \text{or} \quad \times\gamma_{jl}$$

$$\Rightarrow \quad \partial_i\gamma^{jl} = -\gamma^{jm}\gamma^{kl}\partial_i\gamma_{mk}$$

$$\wedge \quad \partial_i\gamma_{lk} = -\gamma_{mk}\gamma_{jl}\partial_i\gamma^{jm} \,. \tag{G.43}$$

Contracting the first result over i and l gives us

$$\partial_i\gamma^{ji} = -\gamma^{jm}\gamma^{ik}\partial_i\gamma_{mk} \,. \tag{G.44}$$

The contracted Christoffel symbol of the conformal metric is

$$\tilde{\Gamma}^i = \frac{1}{2}\tilde{\gamma}^{mn}\tilde{\gamma}^{il}\left(\partial_m\tilde{\gamma}_{nl} + \partial_n\tilde{\gamma}_{lm} - \partial_l\tilde{\gamma}_{mn}\right) . \tag{G.45}$$

Recalling that $\tilde{\gamma} = 1$ and, hence,

$$\partial_i\tilde{\gamma} = \tilde{\gamma}\,\tilde{\gamma}^{mn}\partial_i\tilde{\gamma}_{mn} = -\tilde{\gamma}\,\tilde{\gamma}_{mn}\partial_i\tilde{\gamma}^{mn} = 0 \,, \tag{G.46}$$

we obtain

$$\tilde{\Gamma}^i = \tilde{\gamma}^{mn}\tilde{\gamma}^{il}\partial_m\tilde{\gamma}_{nl} = -\partial_m\tilde{\gamma}^{mi} \,. \tag{G.47}$$

This also proofs (G.42) since

$$\tilde{\Gamma}^m_{im} = \frac{1}{2}\tilde{\gamma}^{mn}(\partial_i\tilde{\gamma}_{mn} + \partial_m\tilde{\gamma}_{ni} - \partial_n\tilde{\gamma}_{im}) = \frac{1}{2}\tilde{\gamma}^{mn}\partial_i\tilde{\gamma}_{mn} + 0 + 0 = 0 \,. \tag{G.48}$$

□

Proposition: The ADM equations (F.96)-(F.99) together with the definition of the variable $\tilde{\Gamma}^i$ in Eq. (G.36) result in the BSSNOK equation,

$$\mathcal{H} = \mathcal{R} - \tilde{A}^{mn}\tilde{A}_{mn} + \frac{2}{3}K^2 - 2\Lambda - 16\pi\rho = 0\,, \tag{G.49}$$

$$\mathcal{M}_i = \frac{2}{3}\partial_i K - \tilde{\gamma}^{mn}\tilde{D}_m\tilde{A}_{in} + \frac{3}{2}\tilde{A}_i{}^m\frac{\partial_m\chi}{\chi} + 8\pi j_i = 0\,, \tag{G.50}$$

$$\partial_t\chi = \beta^m\partial_m\chi - \frac{2}{3}\chi\partial_m\beta^m + \frac{2}{3}\alpha\chi K\,, \tag{G.51}$$

$$\partial_t\tilde{\gamma}_{ij} = \beta^m\partial_m\tilde{\gamma}_{ij} + 2\tilde{\gamma}_{m(i}\partial_{j)}\beta^m - \frac{2}{3}\tilde{\gamma}_{ij}\partial_m\beta^m - 2\alpha\tilde{A}_{ij}\,, \tag{G.52}$$

$$\partial_t K = \beta^m\partial_m K - \chi\tilde{\gamma}^{mn}D_mD_n\alpha + \alpha\left[\tilde{A}^{mn}\tilde{A}_{mn} + \frac{1}{3}K^2 - \Lambda + 4\pi(S+\rho)\right]\,, \tag{G.53}$$

$$\begin{aligned}\partial_t\tilde{A}_{ij} &= \beta^m\partial_m\tilde{A}_{ij} + 2\tilde{A}_{m(i}\partial_{j)}\beta^m - \frac{2}{3}\tilde{A}_{ij}\partial_m\beta^m + \alpha K\tilde{A}_{ij} - 2\alpha\tilde{A}_{im}\tilde{A}^m{}_j \\ &\quad + \chi\left(\alpha\mathcal{R}_{ij} - D_iD_j\alpha - 8\pi S_{ij}\right)^{\mathrm{TF}}\,,\end{aligned} \tag{G.54}$$

$$\begin{aligned}\partial_t\tilde{\Gamma}^i &= \beta^m\partial_m\tilde{\Gamma}^i - \tilde{\Gamma}^m\partial_m\beta^i + \frac{2}{3}\tilde{\Gamma}^i\partial_m\beta^m + \tilde{\gamma}^{mn}\partial_m\partial_n\beta^i + \frac{1}{3}\tilde{\gamma}^{im}\partial_m\partial_n\beta^n + 2\alpha\tilde{\Gamma}^i_{mn}\tilde{A}^{mn} \\ &\quad - 2\tilde{A}^{im}\partial_m\alpha - \frac{4}{3}\alpha\tilde{\gamma}^{im}\partial_m K - 3\alpha\tilde{A}^{im}\frac{\partial_m\chi}{\chi} - 16\pi\alpha\tilde{\gamma}^{im}j_m - \sigma\mathcal{G}^i\,,\end{aligned} \tag{G.55}$$

where in the last expression σ is a parameter and $\mathcal{G}^i$ the auxiliary constraint from Eq. (G.37).

The derivation of these expressions is lengthy; we therefore mention some comments while our memory is still fresh before we risk its erasure in the proof's odyssey.

- The Hamiltonian and momentum constraints (G.49), (G.50) are not employed in the time evolution, but merely serve as a diagnostic; if they are not satisfied with high precision during the evolution, something has gone wrong. Evolutions that do not employ the constraints are commonly called *free evolutions* in contrast to *constrained evolutions* where the constraints are actively used in the update of variables and thereby replace some of the time evolution equations. All 3+1 evolutions we are aware of are free evolutions, since the repeated solving of the constraints at every time step is computationally very expensive.
- The free parameter σ in Eq. (G.55) needs to be positive to obtain stable evolutions; this is most likely due to the fact that with $\sigma > 0$, this term damps violations of the auxiliary constraint $\mathcal{G}^i$ whereas for $\sigma < 0$ such violations are enhanced. Alternatively to adding the $\sigma\mathcal{G}^i$ term, empirical studies have shown that stable evolutions can also be obtained by replacing in Eq. (G.55) all occurrences of undifferentiated $\tilde{\Gamma}^i$ with their definition in terms

of the metric $\tilde{\gamma}_{ij} = \tilde{\gamma}^{mn}\tilde{\Gamma}^{i}_{mn} = \ldots$ [30].

- It has also been found empirically that the auxiliary constraints $\tilde{A}^{m}{}_{m} = 0$ needs to be enforced at regular intervals. This is easy to achieve by replacing

$$\tilde{A}_{ij} \to \tilde{A}_{ij} - \frac{1}{3}\tilde{\gamma}_{ij}\tilde{A}^{m}{}_{m}\,. \tag{G.56}$$

  Note that algebraic constraints are much easier to enforce than differential constraints like $\mathcal{H}$. All codes we are aware of enforce Eq. (G.56) at each time step.

- The second auxiliary constraint $\det\tilde{\gamma}_{ij} = 1$, in contrast, does not appear to require manual enforcement. Most codes we are aware of, have this optionally implemented, but there have been no reports where this enforcement has been found necessary to cure instabilities.

Proof. (1) We begin with the Hamiltonian constraint (G.49). Using

$$\begin{aligned} K^{mn}K_{mn} &= \gamma^{mk}\gamma^{nl}K_{kl}K_{mn} = \chi^2\tilde{\gamma}^{mk}\tilde{\gamma}^{nl}\frac{1}{\chi^2}\left(\tilde{A}_{kl} + \frac{1}{3}\tilde{\gamma}_{kl}K\right)\left(\tilde{A}_{mn} + \frac{1}{3}\tilde{\gamma}_{mn}K\right) \\ &= \tilde{A}^{mn}\tilde{A}_{mn} + \frac{2}{3}\tilde{\gamma}^{kl}K\tilde{A}_{kl} + \frac{1}{9}\tilde{\gamma}^{kl}\tilde{\gamma}_{kl}K^2 = \tilde{A}^{mn}\tilde{A}_{mn} + 0 + \frac{1}{3}K^2\,, \end{aligned} \tag{G.57}$$

the ADM version (F.96) becomes

$$\mathcal{H} = \mathcal{R} + K^2 - K_{mn}K^{mn} - 2\Lambda - 16\pi\rho = \mathcal{R} + \frac{2}{3}K^2 - \tilde{A}^{mn}\tilde{A}_{mn} - 2\Lambda - 16\pi\rho\,. \tag{G.58}$$

(2) For the momentum constraint (G.50), we define $A_{ij} \coloneqq K_{ij} - \frac{1}{3}\gamma_{ij}K = \tilde{A}_{ij}\chi^{-1}$ which gives us

$$\begin{aligned} \gamma^{mn}D_mA_{in} &= \gamma^{mn}\left(\partial_mA_{in} - \Gamma^{l}_{im}A_{ln} - \Gamma^{l}_{nm}A_{il}\right) \\ &= \gamma^{mn}\Bigg[\frac{1}{\chi}\partial_m\tilde{A}_{in} - \tilde{A}_{in}\frac{\partial_m\chi}{\chi^2} - \frac{1}{\chi}\tilde{\Gamma}^{l}_{im}\tilde{A}_{ln} - \frac{1}{\chi}\tilde{\Gamma}^{l}_{nm}\tilde{A}_{il} \\ &\qquad + \frac{1}{2\chi}\left(\delta^{l}{}_{m}\partial_i\chi + \delta^{l}{}_{i}\partial_m\chi - \tilde{\gamma}_{im}\tilde{\gamma}^{lk}\partial_k\chi\right)\frac{\tilde{A}_{ln}}{\chi} \\ &\qquad + \frac{1}{2\chi}\left(\delta^{l}{}_{m}\partial_n\chi + \delta^{l}{}_{n}\partial_m\chi - \tilde{\gamma}_{nm}\tilde{\gamma}^{lk}\partial_k\chi\right)\frac{\tilde{A}_{il}}{\chi}\Bigg] \\ &= \tilde{\gamma}^{mn}\tilde{D}_m\tilde{A}_{in} + \frac{\tilde{\gamma}^{mn}}{2\chi}\left(\tilde{A}_{mn}\partial_i\chi + \tilde{A}_{in}\partial_m\chi\right) - \frac{1}{2\chi}\left(\delta^{n}{}_{i}\tilde{\gamma}^{lk}\partial_k\chi\tilde{A}_{ln} + 3\tilde{\gamma}^{lk}\partial_k\chi\tilde{A}_{il}\right) \\ &= \tilde{\gamma}^{mn}\tilde{D}_m\tilde{A}_{in} + \frac{1}{2\chi}\left(0 + \tilde{A}_i{}^{m}\partial_m\chi - \tilde{A}^{k}{}_{i}\partial_k\chi - 3\tilde{A}_i{}^{k}\partial_k\chi\right) \end{aligned}$$

$$= \tilde{\gamma}^{mn}\tilde{D}_m\tilde{A}_{in} - \frac{3}{2}\tilde{A}_i{}^m\frac{\partial_m\chi}{\chi}\,. \tag{G.59}$$

It follows that

$$D_mK_i{}^m = \gamma^{mn}D_mK_{in} = \gamma^{mn}\left(D_mA_{in} + \frac{1}{3}\gamma_{in}D_mK\right) = \gamma^{mn}D_mA_{in} + \frac{1}{3}D_iK\,, \tag{G.60}$$

and therefore

$$\mathcal{M}_i = D_iK - D_mK_i{}^m + 8\pi j_i = \frac{2}{3}\underbrace{D_iK}_{=\partial_i K} - \tilde{\gamma}^{mn}\tilde{D}_m\tilde{A}_{in} + \frac{3}{2}\tilde{A}_i{}^m\frac{\partial_m\chi}{\chi} + 8\pi j_i = 0\,. \tag{G.61}$$

(3) Next, we consider the evolution equation (G.51) for the conformal factor χ. Using Eq. (G.30) for the spatial metric γ_{ij} together with chain rule and the definition of χ gives us

$$\partial_i\chi = \partial_i\gamma^{-1/3} = -\frac{1}{3}\gamma^{-4/3}\partial_i\gamma = -\frac{1}{3}\gamma^{-4/3}\gamma\gamma^{mn}\partial_i\gamma_{mn} = -\frac{1}{3}\chi\gamma^{mn}\partial_i\gamma_{mn}\,, \tag{G.62}$$

and likewise for $\partial_t\gamma$. We then multiply Eq. (F.98) with γ^{ij} and obtain

$$-\frac{3}{\chi}\partial_t\chi = -\frac{3}{\chi}\beta^m\partial_m\chi + 2\partial_m\beta^m - 2\alpha K$$

$$\Rightarrow\quad \partial_t\chi = \beta^m\partial_m\chi - \frac{2}{3}\chi\partial_m\beta^m + \frac{2}{3}\alpha\chi K\,. \tag{G.63}$$

(4) The evolution equation (G.52) for $\tilde{\gamma}_{ij}$ also follows from Eq. (F.98). Chain rule gives us for $\gamma_{ij} = \tilde{\gamma}_{ij}/\chi$

$$\partial\gamma_{ij} = \frac{1}{\chi}\partial\tilde{\gamma}_{ij} - \frac{\tilde{\gamma}_{ij}}{\chi^2}\partial\chi\,,$$

so that Eq. (F.98) becomes

$$\begin{aligned}
\partial_t\tilde{\gamma}_{ij} &= \beta^m\partial_m\tilde{\gamma}_{ij} + \frac{\tilde{\gamma}_{ij}}{\chi}\left(\partial_t\chi - \beta^m\partial_m\chi\right) + 2\tilde{\gamma}_{m(i}\partial_{j)}\beta^m - 2\alpha\chi\frac{1}{\chi}\left(\tilde{A}_{ij} + \frac{1}{3}\tilde{\gamma}_{ij}K\right) \\
&\overset{(G.63)}{=} \beta^m\partial_m\tilde{\gamma}_{ij} + \frac{\tilde{\gamma}_{ij}}{\chi}\left(\frac{2}{3}\alpha\chi K - \frac{2}{3}\chi\partial_m\beta^m\right) + 2\tilde{\gamma}_{m(i}\partial_{j)}\beta^m - 2\alpha\tilde{A}_{ij} - \frac{2}{3}\tilde{\gamma}_{ij}\alpha K \\
&= \beta^m\partial_m\tilde{\gamma}_{ij} + 2\tilde{\gamma}_{m(i}\partial_{j)}\beta^m - \frac{2}{3}\tilde{\gamma}_{ij}\partial_m\beta^m - 2\alpha\tilde{A}_{ij}\,.
\end{aligned} \tag{G.64}$$

(5) For the trace of the extrinsic curvature, we will use the relations (G.40),

$$\partial\gamma_{ij} = -\gamma_{im}\gamma_{jn}\partial\gamma^{mn}\,, \qquad \partial\gamma^{ij} = -\gamma^{im}\gamma^{jn}\partial\gamma_{mn}\,,$$

which gives us

$$\partial_t K = \partial_t(\gamma^{ij}K_{ij}) = \gamma^{ij}\partial_t K_{ij} + K_{ij}\partial_t\gamma^{ij} = \gamma^{ij}\partial_t K_{ij} - K_{ij}\gamma^{im}\gamma^{jn}\partial_t\gamma_{mn} = \gamma^{ij}\partial_t K_{ij} - K^{ij}\partial_t\gamma_{ij}\,.$$

Together with Eqs. (F.98) and (F.99) we obtain

$$\begin{aligned}
\partial_t K &= \gamma^{ij}\beta^m\partial_m K_{ij} + 2\gamma^{ij}K_{m(i}\partial_{j)}\beta^m - \gamma^{ij}D_iD_j\alpha + \alpha(\mathcal{R} + K^2 - 2K^{mn}K_{mn}) \\
&\quad -3\alpha\Lambda - 8\pi\alpha\left[S - \frac{3}{2}(S-\rho)\right] - K^{ij}\left[\beta^m\partial_m\gamma_{ij} + 2\gamma_{m(i}\partial_{j)}\beta^m - 2\alpha K_{ij}\right] \\
&= \beta^m\gamma^{ij}\partial_m K_{ij} - \beta^m K^{ij}\left(-\gamma_{ik}\gamma_{jl}\partial_m\gamma^{kl}\right) + \alpha(\mathcal{R}+K^2) - 3\alpha\Lambda + 4\pi\alpha(S-3\rho) \\
&\quad -\gamma^{ij}D_iD_j\alpha + \gamma^{ij}K_{mi}\partial_j\beta^m + \gamma^{ij}K_{mj}\partial_i\beta^m - K^{ij}\gamma_{mi}\partial_j\beta^m - K^{ij}\gamma_{mj}\partial_i\beta^m \\
&= \beta^m\gamma^{ij}\partial_m K_{ij} + \beta^m K_{ij}\partial_m\gamma^{ij} + \alpha(\mathcal{R}+K^2) - 3\alpha\Lambda + 4\pi\alpha(S-3\rho) - \gamma^{mn}D_mD_n\alpha \\
&= \beta^m\partial_m K + \alpha(\mathcal{R}+K^2) - 3\alpha\Lambda + 4\pi\alpha(S-3\rho) - \chi\tilde{\gamma}^{mn}D_mD_n\alpha\,. \qquad \text{(G.65)}
\end{aligned}$$

Next, we subtract α times the Hamiltonian constraint (G.49),

$$\mathcal{H} = \mathcal{R} + \frac{2}{3}K^2 - \tilde{A}^{mn}\tilde{A}_{mn} - 2\Lambda - 16\pi\rho\,,$$

which is zero. Note that this addition changes the principal part of the PDE system and also also enables us to feed back any constraint violations (which are inevitable in a numerical implementation) into the evolution of the variables. Done the "right" way, this may damp constraint violations and also facilitate the propagation of constraint violating modes off the computational domain. In practice, finding the right way often involves some trial and error. For our equation we obtain

$$\partial_t K = \beta^m\partial_m K - \chi\tilde{\gamma}^{mn}D_mD_n\alpha + \alpha\left[\tilde{A}^{mn}\tilde{A}_{mn} + \frac{1}{3}K^2 - \Lambda + 4\pi(S+\rho)\right]. \qquad \text{(G.66)}$$

(6) For the traceless extrinsic curvature,

$$\tilde{A}_{ij} = \chi K_{ij} - \frac{1}{3}\tilde{\gamma}_{ij}K\,, \qquad \text{(G.67)}$$

we note that for a derivative operator ∂,

$$\partial\tilde{A}_{ij} = K_{ij}\partial\chi + \chi\partial K_{ij} - \frac{1}{3}K\partial\tilde{\gamma}_{ij} - \frac{1}{3}\tilde{\gamma}_{ij}\partial K\,. \qquad \text{(G.68)}$$

Applying this for the time derivative, we can insert using Eq. (G.51) for $\partial_t\chi$, Eq. (F.99) for $\partial_t K_{ij}$ and Eq. (G.52) for $\partial_t\tilde{\gamma}_{ij}$. For $\partial_t K$, however, it turns out more convenient to use the intermediate result (G.65) without subtraction of the Hamiltonian constraint. The rest is lengthy but straightforward algebra leading to

$$
\begin{aligned}
\partial_t \tilde{A}_{ij} &= K_{ij}\left\{\beta^m\partial_m\chi - \frac{2}{3}\chi\partial_m\beta^m + \frac{2}{3}\alpha\chi K\right\} + \chi\Big\{\beta^m\partial_m K_{ij} + 2K_{m(i}\partial_{j)}\beta^m - D_iD_j\alpha \\
&\quad +\alpha\left(\mathcal{R}_{ij} + KK_{ij} - 2K_{im}K^m{}_j\right) - \alpha\Lambda\gamma_{ij} - 8\pi\alpha\left[S_{ij} - \frac{1}{2}\gamma_{ij}(S-\rho)\right]\Big\} \\
&\quad -\frac{1}{3}K\left\{\beta^m\partial_m\tilde{\gamma}_{ij} + 2\tilde{\gamma}_{m(i}\partial_{j)}\beta^m - \frac{2}{3}\tilde{\gamma}_{ij}\partial_m\beta^m - 2\alpha\tilde{A}_{ij}\right\} \\
&\quad -\frac{1}{3}\tilde{\gamma}_{ij}\left\{\beta^m\partial_m K - \chi\tilde{\gamma}^{mn}D_mD_n\alpha + \alpha\left[\mathcal{R} + K^2 - 3\Lambda + 4\pi(S-3\rho)\right]\right\} \\
&= \beta^m\left\{K_{ij}\partial_m\chi + \chi\partial_m K_{ij} - \frac{1}{3}K\partial_m\tilde{\gamma}_{ij} - \frac{1}{3}\tilde{\gamma}_{ij}\partial_m K\right\} + \partial_m\beta^m\left\{-\frac{2}{3}\chi K_{ij} + \frac{2}{9}K\tilde{\gamma}_{ij}\right\} \\
&\quad -\chi\left\{D_iD_j\alpha - \frac{1}{3}\tilde{\gamma}_{ij}\tilde{\gamma}^{mn}D_mD_n\alpha\right\} + \alpha\left\{\chi\mathcal{R}_{ij} - \frac{1}{3}\tilde{\gamma}_{ij}\mathcal{R}\right\} \\
&\quad +2\chi\left[K_{m(i}\partial_{j)} - \frac{1}{3}K\gamma_{m(i}\partial_{j)}\right]\beta^m + 4\pi\chi\alpha\left\{-2S_{ij} + \gamma_{ij}(S-\rho) - \frac{1}{3}\gamma_{ij}(S-3\rho)\right\} \\
&\quad +\frac{2}{3}\alpha\chi KK_{ij} + \chi\alpha KK_{ij} - 2\chi\alpha K_{im}K^m{}_j + \frac{2}{3}K\alpha\tilde{A}_{ij} - \frac{1}{3}\tilde{\gamma}_{ij}\alpha K^2 \\
&= \beta^m\partial_m\tilde{A}_{ij} - \frac{2}{3}\chi\left(K_{ij} - \frac{1}{3}\gamma_{ij}K\right)\partial_m\beta^m - \chi(D_iD_j\alpha)^{\mathrm{TF}} + \alpha\chi\mathcal{R}^{\mathrm{TF}}_{ij} + 2\tilde{A}_{m(i}\partial_{j)}\beta^m \\
&\quad +4\pi\chi\alpha\left(-2S_{ij} + \frac{2}{3}\gamma_{ij}S + 0\right) + \underbrace{\frac{5}{3}\alpha\chi KK_{ij} - 2\alpha\chi K_{im}K^m{}_j + \frac{2}{3}\alpha K\tilde{A}_{ij} - \frac{1}{3}\tilde{\gamma}_{ij}\alpha K^2}_{=:X_{ij}},
\end{aligned}
$$

where 'TF' denotes the tracefree part. The last four terms simplify to

$$
\begin{aligned}
X_{ij} &= \frac{5}{3}\alpha K\left(\tilde{A}_{ij} + \frac{1}{3}\tilde{\gamma}_{ij}K\right) - 2\alpha\left(\tilde{A}_{im} + \frac{1}{3}\tilde{\gamma}_{im}K\right)\left(\tilde{A}^m{}_j + \frac{1}{3}\delta^m{}_jK\right) + \frac{2}{3}\alpha K\tilde{A}_{ij} - \frac{1}{3}\tilde{\gamma}_{ij}\alpha K^2 \\
&= \frac{5}{3}\alpha K\tilde{A}_{ij} + \frac{5}{9}\alpha\tilde{\gamma}_{ij}K^2 - 2\alpha\tilde{A}_{im}\tilde{A}^m{}_j - \frac{4}{3}\alpha\tilde{A}_{ij}K - \frac{2}{9}\tilde{\gamma}_{ij}K^2 + \frac{2}{3}\alpha K\tilde{A}_{ij} - \frac{1}{3}\tilde{\gamma}_{ij}\alpha K^2 \\
&= \alpha K\tilde{A}_{ij} - 2\alpha\tilde{A}_{im}\tilde{A}^m{}_j\,,
\end{aligned}
$$

so that

$$
\begin{aligned}
\partial_t\tilde{A}_{ij} &= \beta^m\partial_m\tilde{A}_{ij} + 2\tilde{A}_{m(i}\partial_{j)}\beta^m - \frac{2}{3}\tilde{A}_{ij}\partial_m\beta^m + \chi\left[\alpha\mathcal{R}_{ij} - D_iD_j\alpha - 8\pi S_{ij}\right]^{\mathrm{TF}} \\
&\quad +\alpha K\tilde{A}_{ij} - 2\alpha\tilde{A}_{im}\tilde{A}^m{}_j\,. \qquad \text{(G.69)}
\end{aligned}
$$

(7) The evolution equation for $\tilde{\Gamma}^i$ is the lengthiest derivation and requires the auxiliary relations (G.40), (G.41) as well as $\partial_i\tilde{\gamma} = \tilde{\gamma}^{mn}\partial_i\tilde{\gamma}_{mn} = 0$. Our strategy is to start with (G.41),

$$
\begin{aligned}
& \tilde{\Gamma}^i = \tilde{\gamma}^{mn}\tilde{\gamma}^{il}\partial_m\tilde{\gamma}_{nl} \\
\Rightarrow\quad & \partial_t\tilde{\Gamma}^i = \tilde{\gamma}^{il}\partial_m\tilde{\gamma}_{nl}\partial_t\tilde{\gamma}^{mn} + \tilde{\gamma}^{mn}\partial_m\tilde{\gamma}_{nl}\partial_t\tilde{\gamma}^{il} + \tilde{\gamma}^{mn}\tilde{\gamma}^{il}\partial_m(\partial_t\tilde{\gamma}_{nl}) \qquad \text{(G.70)} \\
\Rightarrow\quad & \partial_t\tilde{\Gamma}^i = -\tilde{\gamma}^{il}\partial_m\tilde{\gamma}_{nl}\tilde{\gamma}^{mj}\tilde{\gamma}^{nk}\partial_t\tilde{\gamma}_{jk} - \tilde{\gamma}^{mn}\partial_m\tilde{\gamma}_{nl}\tilde{\gamma}^{ij}\tilde{\gamma}^{kl}\partial_t\tilde{\gamma}_{jk} \\
& \qquad + \tilde{\gamma}^{mn}\tilde{\gamma}^{il}\partial_m\left[\beta^k\partial_k\tilde{\gamma}_{nl} + 2\tilde{\gamma}_{k(n}\partial_{l)}\beta^k - \frac{2}{3}\tilde{\gamma}_{nl}\partial_k\beta^k - 2\alpha\tilde{A}_{nl}\right], \qquad \text{(G.71)}
\end{aligned}
$$

where in the last line, we have substituted for $\partial_t\tilde{\gamma}_{nl}$ using the evolution equation (G.52). We will likewise substitute for the other time derivatives of the metric. Note, however, that Eq. (G.70) also holds for spatial derivatives ∂_k and we will use the reverse relation to reconstruct $\partial_k\tilde{\Gamma}^i$ terms from the spatial derivatives of the metric. In this process, we will mark terms by underlining in different styles to better follow how they are combined or cancel. We then obtain

$$
\begin{aligned}
\partial_t\tilde{\Gamma}^i \;=\; & -\tilde{\gamma}^{il}\partial_m\tilde{\gamma}_{nl}\tilde{\gamma}^{mj}\tilde{\gamma}^{nk}\left[\underline{\beta^r\partial_r\tilde{\gamma}_{jk}} + 2\tilde{\gamma}_{r(j}\partial_{k)}\beta^r - \frac{2}{3}\tilde{\gamma}_{jk}\partial_r\beta^r - 2\alpha\tilde{A}_{jk}\right] \\
& -\tilde{\gamma}^{mn}\partial_m\tilde{\gamma}_{nl}\tilde{\gamma}^{ij}\tilde{\gamma}^{kl}\left[\underline{\beta^r\partial_r\tilde{\gamma}_{jk}} + 2\tilde{\gamma}_{r(j}\partial_{k)}\beta^r - \frac{2}{3}\tilde{\gamma}_{jk}\partial_r\beta^r - 2\alpha\tilde{A}_{jk}\right] \\
& +\tilde{\gamma}^{mn}\tilde{\gamma}^{il}\left[\underline{\beta^k\partial_m(\partial_k\tilde{\gamma}_{nl})} + \partial_k\tilde{\gamma}_{nl}\partial_m\beta^k\right] \\
& +\tilde{\gamma}^{mn}\tilde{\gamma}^{il}\partial_m\left[\tilde{\gamma}_{kn}\partial_l\beta^k + \tilde{\gamma}_{kl}\partial_n\beta^k - \frac{2}{3}\tilde{\gamma}_{nl}\partial_k\beta^k - 2\alpha\tilde{A}_{nl}\right] \\
=\; & \underline{\tilde{\gamma}^{il}\partial_m\tilde{\gamma}_{nl}\beta^r\partial_r\tilde{\gamma}^{mn} + \tilde{\gamma}^{mn}\partial_m\tilde{\gamma}_{nl}\beta^r\partial_r\tilde{\gamma}^{il} + \tilde{\gamma}^{mn}\tilde{\gamma}^{il}\beta^k\partial_m\partial_k\tilde{\gamma}_{nl}} \\
& +\partial_r\beta^r\left(\frac{2}{3}\tilde{\gamma}^{il}\partial_m\tilde{\gamma}_{nl}\tilde{\gamma}^{mn} + \frac{2}{3}\tilde{\gamma}^{mn}\partial_m\tilde{\gamma}_{nl}\tilde{\gamma}^{il} - \frac{2}{3}\tilde{\gamma}^{mn}\tilde{\gamma}^{il}\partial_m\tilde{\gamma}_{nl}\right) - \frac{2}{3}\tilde{\gamma}^{mn}\tilde{\gamma}^{il}\tilde{\gamma}_{nl}\partial_m\partial_k\beta^k \\
& +\partial_m\tilde{\gamma}^{ik}\tilde{\gamma}^{mj}(\tilde{\gamma}_{rj}\partial_k\beta^r + \tilde{\gamma}_{rk}\partial_j\beta^r) - \tilde{\Gamma}^k\tilde{\gamma}^{ij}(\tilde{\gamma}_{rj}\partial_k\beta^r + \tilde{\gamma}_{rk}\partial_j\beta^r) - \partial_k\tilde{\gamma}^{mi}\partial_m\beta^k \\
& +\tilde{\gamma}^{mn}\tilde{\gamma}^{il}\left[\partial_m\tilde{\gamma}_{kn}\partial_l\beta^k + \tilde{\gamma}_{kn}\partial_m\partial_l\beta^k + \partial_m\tilde{\gamma}_{kl}\partial_n\beta^k + \tilde{\gamma}_{kl}\partial_m\partial_n\beta^k\right] \\
& +2\alpha\tilde{\gamma}^{il}\partial_m\tilde{\gamma}_{nl}\tilde{A}^{mn} + 2\alpha\tilde{\gamma}^{mn}\partial_m\tilde{\gamma}_{nl}\tilde{A}^{il} - 2\tilde{\gamma}^{mn}\tilde{\gamma}^{il}\left[\tilde{A}_{nl}\partial_m\alpha + \alpha\partial_m\tilde{A}_{nl}\right]
\end{aligned}
$$

$$
\begin{aligned}
&= \beta^r\partial_r\tilde{\Gamma}^i + \frac{2}{3}\partial_r\beta^r\tilde{\Gamma}^i - \frac{2}{3}\tilde{\gamma}^{mi}\partial_m\partial_k\beta^k + \tilde{\gamma}^{il}\partial_k\partial_l\beta^k + \tilde{\gamma}^{mn}\partial_m\partial_n\beta^i + \partial_m\tilde{\gamma}^{ik}\partial_k\beta^m \\
&\quad + \tilde{\gamma}^{mj}\partial_m\tilde{\gamma}^{ik}\tilde{\gamma}_{rk}\partial_j\beta^r - \tilde{\Gamma}^k\partial_k\beta^i - \tilde{\Gamma}^k\tilde{\gamma}^{ij}\tilde{\gamma}_{rk}\partial_j\beta^r + \tilde{\gamma}^{mn}\tilde{\gamma}^{il}\partial_m\tilde{\gamma}_{kn}\partial_l\beta^k + \tilde{\gamma}^{mn}\tilde{\gamma}^{il}\partial_m\tilde{\gamma}_{kl}\partial_n\beta^k \\
&\quad - \partial_k\tilde{\gamma}^{mi}\partial_m\beta^k + 2\alpha\left[\tilde{\gamma}^{il}\partial_m\tilde{\gamma}_{nl}\tilde{A}^{mn} + \tilde{\gamma}^{mn}\partial_m\tilde{\gamma}_{nl}\tilde{A}^{il} - \tilde{A}^{im}\frac{\partial_m\alpha}{\alpha} - \tilde{\gamma}^{mn}\tilde{\gamma}^{il}\partial_m\tilde{A}_{nl}\right] \\
&= \beta^m\partial_m\tilde{\Gamma}^i + \frac{2}{3}\partial_m\beta^m\tilde{\Gamma}^i + \frac{1}{3}\tilde{\gamma}^{il}\partial_k\partial_l\beta^k + \tilde{\gamma}^{mn}\partial_m\partial_n\beta^i - \tilde{\Gamma}^k\partial_k\beta^i - \tilde{\gamma}^{mj}\tilde{\gamma}^{il}\tilde{\gamma}^{kn}\partial_m\tilde{\gamma}_{ln}\tilde{\gamma}_{rk}\partial_j\beta^r \\
&\quad - \tilde{\gamma}^{mn}\tilde{\gamma}^{kl}\partial_m\tilde{\gamma}_{nl}\tilde{\gamma}^{ij}\tilde{\gamma}_{rk}\partial_j\beta^r + \tilde{\gamma}^{mn}\tilde{\gamma}^{il}\partial_m\tilde{\gamma}_{kn}\partial_l\beta^k + \tilde{\gamma}^{mn}\tilde{\gamma}^{il}\partial_m\tilde{\gamma}_{kl}\partial_n\beta^k - 2\tilde{A}^{im}\partial_m\alpha \\
&\quad - 2\alpha\left[\tilde{\gamma}^{mn}\tilde{\gamma}^{il}\partial_m\tilde{A}_{nl} - \tilde{\gamma}^{il}\partial_m\tilde{\gamma}_{nl}\tilde{A}^{mn} - \tilde{\gamma}^{mn}\partial_m\tilde{\gamma}_{nl}\tilde{A}^{il}\right] \\
&= \beta^m\partial_m\tilde{\Gamma}^i + \frac{2}{3}\tilde{\Gamma}^i\partial_m\beta^m + \frac{1}{3}\tilde{\gamma}^{im}\partial_m\partial_n\beta^n + \tilde{\gamma}^{mn}\partial_m\partial_n\beta^i - \tilde{\Gamma}^m\partial_m\beta^i - 2\tilde{A}^{im}\partial_m\alpha \\
&\quad - \tilde{\gamma}^{mj}\tilde{\gamma}^{il}\partial_m\tilde{\gamma}_{ln}\partial_j\beta^n - \tilde{\gamma}^{mn}\tilde{\gamma}^{ij}\partial_m\tilde{\gamma}_{nl}\partial_j\beta^l + \tilde{\gamma}^{mn}\tilde{\gamma}^{il}\partial_m\tilde{\gamma}_{kn}\partial_l\beta^k + \tilde{\gamma}^{mn}\tilde{\gamma}^{il}\partial_m\tilde{\gamma}_{kl}\partial_n\beta^k \\
&\quad - 2\alpha\left[\tilde{\gamma}^{mn}\tilde{\gamma}^{il}\partial_m\tilde{A}_{nl} - \tilde{\gamma}^{il}\partial_m\tilde{\gamma}_{nl}\tilde{A}^{mn} - \tilde{\gamma}^{mn}\partial_m\tilde{\gamma}_{nl}\tilde{A}^{il}\right]\,.
\end{aligned} \tag{G.72}
$$

The last line can be written as a covariant derivative (here we need $\tilde{\gamma}^{mn}\partial_i\tilde{\gamma}_{mn} = 0$),

$$
\begin{aligned}
\tilde{D}_m\tilde{A}_{nl} &= \partial_m\tilde{A}_{nl} - \tilde{\Gamma}^r_{nm}\tilde{A}_{rl} - \tilde{\Gamma}^r_{lm}\tilde{A}_{nr} \\
&= \partial_m\tilde{A}_{nl} - \frac{1}{2}\tilde{\gamma}^{rk}(\partial_n\tilde{\gamma}_{mk} + \partial_m\tilde{\gamma}_{kn} - \partial_k\tilde{\gamma}_{nm})\tilde{A}_{rl} - \frac{1}{2}\tilde{\gamma}^{rk}(\partial_l\tilde{\gamma}_{mk} + \partial_m\tilde{\gamma}_{kl} - \partial_k\tilde{\gamma}_{lm})\tilde{A}_{nr}
\end{aligned}
$$

$$
\begin{aligned}
\Rightarrow\quad \tilde{\gamma}^{mn}\tilde{\gamma}^{il}\tilde{D}_m\tilde{A}_{nl} &= \tilde{\gamma}^{mn}\tilde{\gamma}^{il}\partial_m\tilde{A}_{nl} - \frac{1}{2}\tilde{\gamma}^{mn}(\partial_n\tilde{\gamma}_{mk} + \partial_m\tilde{\gamma}_{kn} - \partial_k\tilde{\gamma}_{nm})\tilde{A}^{ki} \\
&\qquad - \frac{1}{2}\tilde{\gamma}^{il}(\partial_l\tilde{\gamma}_{mk} + \partial_m\tilde{\gamma}_{kl} - \partial_k\tilde{\gamma}_{lm})\tilde{A}^{mk} \\
&= \tilde{\gamma}^{mn}\tilde{\gamma}^{il}\partial_m\tilde{A}_{nl} - \tilde{\gamma}^{mn}\partial_m\tilde{\gamma}_{nk}\tilde{A}^{ki} + 0 - \frac{1}{2}\tilde{\gamma}^{il}(\partial_l\tilde{\gamma}_{mk})\tilde{A}^{mk} \\
&= \tilde{\gamma}^{mn}\tilde{\gamma}^{il}\partial_m\tilde{A}_{nl} - \tilde{\gamma}^{mn}\partial_m\tilde{\gamma}_{nk}\tilde{A}^{ki} - \frac{1}{2}\tilde{\gamma}^{il}(\partial_l\tilde{\gamma}_{mk} - \partial_m\tilde{\gamma}_{kl} - \partial_k\tilde{\gamma}_{lm})\tilde{A}^{mk} - \tilde{\gamma}^{il}\partial_m\tilde{\gamma}_{kl}\tilde{A}^{mk} \\
&= \tilde{\gamma}^{mn}\tilde{\gamma}^{il}\partial_m\tilde{A}_{nl} - \tilde{\gamma}^{mn}\partial_m\tilde{\gamma}_{nk}\tilde{A}^{ki} + \tilde{\Gamma}^i_{mk}\tilde{A}^{mk} - \tilde{\gamma}^{il}\partial_m\tilde{\gamma}_{kl}\tilde{A}^{mk}
\end{aligned}
$$

$$
\Rightarrow\quad \tilde{\gamma}^{mn}\tilde{\gamma}^{il}\partial_m\tilde{A}_{nl} - \tilde{\gamma}^{mn}\partial_m\tilde{\gamma}_{nk}\tilde{A}^{ki} - \tilde{\gamma}^{il}\partial_m\tilde{\gamma}_{kl}\tilde{A}^{mk} = \tilde{\gamma}^{mn}\tilde{\gamma}^{il}\tilde{D}_m\tilde{A}_{nl} - \tilde{\Gamma}^i_{mn}\tilde{A}^{mn}\,.
$$

The left-hand side equals the terms in brackets on the last line of Eq. (G.72) which we can therefore substitute,

$$\begin{aligned}\partial_t\tilde{\Gamma}^i &= \beta^m\partial_m\tilde{\Gamma}^i + \frac{2}{3}\tilde{\Gamma}^i\partial_m\beta^m + \frac{1}{3}\tilde{\gamma}^{im}\partial_m\partial_n\beta^n + \tilde{\gamma}^{mn}\partial_m\partial_n\beta^i - \tilde{\Gamma}^m\partial_m\beta^i - 2\tilde{A}^{im}\partial_m\alpha \\ &\quad -2\alpha\tilde{\gamma}^{mn}\tilde{\gamma}^{il}\tilde{D}_m\tilde{A}_{nl} + 2\alpha\Gamma^i_{mn}\tilde{A}^{mn}\,. \qquad \text{(G.73)}\end{aligned}$$

For the final version, we use the momentum constraint (G.50) in the form,

$$\tilde{\gamma}^{il}\tilde{\gamma}^{mn}\tilde{D}_m\tilde{A}_{nl} = \frac{2}{3}\tilde{\gamma}^{il}\partial_l K + \frac{3}{2}\tilde{A}^{im}\frac{\partial_m\chi}{\chi} + 8\pi\tilde{\gamma}^{im}j_m\,, \qquad \text{(G.74)}$$

and subtract $\sigma\mathcal{G}^i$, so that

$$\begin{aligned}\partial_t\tilde{\Gamma}^i &= \beta^m\partial_m\tilde{\Gamma}^i - \tilde{\Gamma}^m\partial_m\beta^i + \frac{2}{3}\tilde{\Gamma}^i\partial_m\beta^m + \frac{1}{3}\tilde{\gamma}^{im}\partial_m\partial_n\beta^n + \tilde{\gamma}^{mn}\partial_m\partial_n\beta^i + 2\alpha\tilde{\Gamma}^i_{mn}\tilde{A}^{mn} \\ &\quad -2\tilde{A}^{im}\partial_m\alpha - \frac{4}{3}\alpha\tilde{\gamma}^{il}\partial_l K - 3\alpha\tilde{A}^{im}\frac{\partial_m\chi}{\chi} - 16\pi\alpha\tilde{\gamma}^{im}j_m - \sigma\mathcal{G}^i\,. \qquad \text{(G.75)}\end{aligned}$$

□

We are not quite done yet; the BSSNOK equations (G.49)-(G.55) contain some auxiliary expressions that we still need to express appropriately in terms of the fundamental variables.

Proposition: The spatial Riemann tensor and second derivative of the lapse function are given by

$$\mathcal{R}_{ij} = \tilde{R}_{ij} + \tilde{R}^{\chi}_{ij}\,, \qquad \text{(G.76)}$$

$$\tilde{\mathcal{R}}_{ij} = -\frac{1}{2}\tilde{\gamma}^{mn}\partial_m\partial_n\tilde{\gamma}_{ij} + \tilde{\gamma}_{m(i}\partial_{j)}\tilde{\Gamma}^m + \tilde{\Gamma}^m\tilde{\Gamma}_{(ij)m} + \tilde{\gamma}^{mn}\tilde{\Gamma}^k_{im}\tilde{\Gamma}_{kjn} + 2\tilde{\gamma}^{mn}\tilde{\Gamma}^k_{m(i}\tilde{\Gamma}_{j)kn}\,,$$

$$\mathcal{R}^{\chi}_{ij} = \frac{1}{2\chi}\left(\tilde{D}_i\tilde{D}_j\chi + \tilde{\gamma}_{ij}\tilde{\gamma}^{mn}\tilde{D}_m\tilde{D}_n\chi\right) - \frac{1}{4\chi^2}\left(\partial_i\chi\partial_j\chi + 3\tilde{\gamma}_{ij}\tilde{\gamma}^{mn}\partial_m\chi\partial_n\chi\right)\,,$$

$$D_iD_j\alpha = \tilde{D}_i\tilde{D}_j\alpha + \frac{1}{\chi}\partial_{(i}\alpha\partial_{j)}\chi - \frac{1}{2\chi}\tilde{\gamma}_{ij}\tilde{\gamma}^{mn}\partial_m\chi\partial_n\alpha\,. \qquad \text{(G.77)}$$

Proof. We start with the Ricci tensor. Writing Eq. (G.38) in the form

$$\Gamma^i_{jk} = \tilde{\Gamma}^i_{jk} - f^i_{jk} \qquad \text{with} \qquad f^i_{jk} = \frac{1}{2\chi}\left(\delta^i{}_k\partial_j\chi + \delta^i{}_j\partial_k\chi - \tilde{\gamma}_{jk}\tilde{\gamma}^{im}\partial_m\chi\right)\,,$$

and recalling that $\tilde{\Gamma}^m_{im} = 0$ by Eq. (G.42), we can write

$$\mathcal{R}_{ij} = \mathcal{R}^m{}_{imj} = \partial_m\Gamma^m_{ij} - \partial_j\Gamma^m_{im} + \Gamma^n_{ij}\Gamma^m_{nm} - \Gamma^n_{im}\Gamma^m_{nj}$$

$$
\begin{aligned}
&= \partial_m \tilde{\Gamma}^m_{ij} - \partial_m f^m_{ij} - \partial_j f^m_{im} - \tilde{\Gamma}^n_{ij} f^m_{nm} + f^n_{ij} f^m_{nm} - \tilde{\Gamma}^n_{im}\tilde{\Gamma}^m_{nj} + f^n_{im}\tilde{\Gamma}^m_{nj} + \tilde{\Gamma}^n_{im} f^m_{nj} - f^n_{im} f^m_{nj} \\
&=: \tilde{\mathcal{R}}_{ij} + \mathcal{R}^\chi_{ij} \,, \qquad \text{(G.78)}
\end{aligned}
$$

with

$$
\begin{aligned}
\tilde{\mathcal{R}}_{ij} &= \partial_k \tilde{\Gamma}^k_{ij} - \tilde{\Gamma}^n_{im}\tilde{\Gamma}^m_{nj} && \text{(G.79)} \\
\mathcal{R}^\chi_{ij} &= -\partial_m f^m_{ij} - \partial_j f^m_{im} - \tilde{\Gamma}^n_{ij} f^m_{nm} + f^n_{ij} f^m_{nm} + f^n_{im}\tilde{\Gamma}^m_{nj} + \tilde{\Gamma}^n_{im} f^m_{nj} - f^n_{im} f^m_{nj} \,. && \text{(G.80)}
\end{aligned}
$$

The conformal Ricci tensor is a good deal harder to rewrite than the two innocent terms might suggest. Recalling Eq. (G.41), we write

$$
\begin{aligned}
\tilde{\gamma}_{mi}\partial_j \tilde{\Gamma}^m = \tilde{\gamma}_{mi}\partial_j \left(\tilde{\gamma}^{ms}\tilde{\gamma}^{kl}\partial_k \tilde{\gamma}_{ls}\right) \\
\tilde{\gamma}_{mi}\tilde{\gamma}^{kl}\partial_j \tilde{\gamma}^{ms}\partial_k \tilde{\gamma}_{ls} + \partial_j \tilde{\gamma}^{kl}\partial_k \tilde{\gamma}_{li} + \tilde{\gamma}^{kl}\partial_j\partial_k \tilde{\gamma}_{li} \\
\Rightarrow \quad \tilde{\gamma}^{km}\partial_k\partial_j \tilde{\gamma}_{mi} = \tilde{\gamma}_{mi}\partial_j \tilde{\Gamma}^m - \tilde{\gamma}_{mi}\tilde{\gamma}^{kl}\partial_j \tilde{\gamma}^{ms}\partial_k \tilde{\gamma}_{ls} - \partial_j \tilde{\gamma}^{kl}\partial_k \tilde{\gamma}_{li} \qquad \text{(G.81)}
\end{aligned}
$$

Defining the Christoffel symbols of the first kind by

$$
\tilde{\Gamma}_{mij} = \tilde{\gamma}_{mn}\tilde{\Gamma}^n_{ij} = \frac{1}{2}\left(\partial_i \tilde{\gamma}_{jm} + \partial_j \tilde{\gamma}_{mi} - \partial_m \tilde{\gamma}_{ij}\right) \qquad \text{(G.82)}
$$

we obtain

$$
\begin{aligned}
\tilde{\mathcal{R}}_{ij} &= \partial_k \left(\tilde{\gamma}^{km}\tilde{\Gamma}_{mij}\right) - \tilde{\Gamma}^n_{im}\tilde{\Gamma}^m_{nj} \;=\; (\partial_k \tilde{\gamma}^{km})\tilde{\Gamma}_{mij} + \tilde{\gamma}^{km}\partial_k \tilde{\Gamma}_{mij} - \tilde{\Gamma}^n_{im}\tilde{\Gamma}^m_{nj} \\
&= \partial_k \tilde{\gamma}^{km}\,\tilde{\Gamma}_{mij} + \frac{1}{2}\tilde{\gamma}^{km}\left(-\partial_k\partial_m \tilde{\gamma}_{ij} + \partial_k\partial_j \tilde{\gamma}_{mi} + \partial_k\partial_i \tilde{\gamma}_{jm}\right) - \tilde{\Gamma}^m_{ik}\tilde{\Gamma}^k_{mj} \\
&\overset{(G.81)}{=} \partial_k \tilde{\gamma}^{km}\,\tilde{\Gamma}_{mij} - \frac{1}{2}\tilde{\gamma}^{km}\partial_k\partial_m \tilde{\gamma}_{ij} + \frac{1}{2}\tilde{\gamma}_{mi}\partial_j \tilde{\Gamma}^m - \frac{1}{2}\tilde{\gamma}_{mi}\tilde{\gamma}^{kl}\partial_j \tilde{\gamma}^{ms}\partial_k \tilde{\gamma}_{ls} - \frac{1}{2}\partial_j \tilde{\gamma}^{kl}\partial_k \tilde{\gamma}_{li} \\
&\quad + \frac{1}{2}\tilde{\gamma}_{mj}\partial_i \tilde{\Gamma}^m - \frac{1}{2}\tilde{\gamma}_{mj}\tilde{\gamma}^{kl}\partial_i \tilde{\gamma}^{ms}\partial_k \tilde{\gamma}_{ls} - \frac{1}{2}\partial_i \tilde{\gamma}^{kl}\partial_k \tilde{\gamma}_{lj} - \tilde{\gamma}^{mn}\tilde{\gamma}^{kl}\tilde{\Gamma}_{nik}\tilde{\Gamma}_{lmj} \qquad \text{(G.83)}
\end{aligned}
$$

Next, we use

$$
-\tilde{\gamma}^{kl}\partial_i \tilde{\gamma}^{ms}\partial_k \tilde{\gamma}_{ls} = \tilde{\gamma}^{kl}\tilde{\gamma}^{mn}\tilde{\gamma}^{sr}\partial_i \tilde{\gamma}_{nr}\,\partial_k \tilde{\gamma}_{ls} = \tilde{\gamma}^{mn}\partial_i \tilde{\gamma}_{nr}(-\partial_k \tilde{\gamma}^{kr}) \overset{(G.40)}{=} \tilde{\gamma}^{mn}\tilde{\Gamma}^r \partial_i \tilde{\gamma}_{nr} \,,
$$

so that

$$
\begin{aligned}
\tilde{\mathcal{R}}_{ij} &= -\frac{1}{2}\tilde{\gamma}^{km}\partial_k\partial_m \tilde{\gamma}_{ij} + \tilde{\gamma}_{m(i}\partial_{j)}\tilde{\Gamma}^m + \partial_k \tilde{\gamma}^{km}\tilde{\Gamma}_{mij} + \frac{1}{2}\tilde{\gamma}_{mi}\tilde{\gamma}^{mn}\tilde{\Gamma}^r \partial_j \tilde{\gamma}_{nr} - \frac{1}{2}\partial_j \tilde{\gamma}^{kl}\partial_k \tilde{\gamma}_{li} \\
&\quad + \frac{1}{2}\tilde{\gamma}_{mj}\tilde{\gamma}^{mn}\tilde{\Gamma}^r \partial_i \tilde{\gamma}_{nr} - \frac{1}{2}\partial_i \tilde{\gamma}^{kl}\partial_k \tilde{\gamma}_{lj} - \tilde{\gamma}^{mn}\tilde{\gamma}^{kl}\tilde{\Gamma}_{nik}\tilde{\Gamma}_{lmj} \,. \qquad \text{(G.84)}
\end{aligned}
$$

We now notice that

$$\tilde{\Gamma}_{(ij)m} = \frac{1}{4}\Big(\partial_j\tilde{\gamma}_{mi} + \partial_m\tilde{\gamma}_{ij} - \partial_i\tilde{\gamma}_{jm} + \partial_i\tilde{\gamma}_{mj} + \partial_m\tilde{\gamma}_{ji} - \partial_j\tilde{\gamma}_{im}\Big) = \frac{1}{2}\partial_m\tilde{\gamma}_{ij}\,, \tag{G.85}$$

$$\partial_k\tilde{\gamma}^{km}\tilde{\Gamma}_{mij} = -\tilde{\Gamma}^m\frac{1}{2}\left(-\partial_m\tilde{\gamma}_{ij} + \partial_i\tilde{\gamma}_{jm} + \partial_j\tilde{\gamma}_{mi}\right)\,, \tag{G.86}$$

which gives us

$$\begin{aligned}\tilde{\mathcal{R}}_{ij} = {} & -\frac{1}{2}\tilde{\gamma}^{km}\partial_k\partial_m\tilde{\gamma}_{ij} + \tilde{\gamma}_{m(i}\partial_{j)}\tilde{\Gamma}^m + \frac{1}{2}\tilde{\Gamma}^m\underbrace{\partial_m\tilde{\gamma}_{ij}}_{=2\tilde{\Gamma}_{(ij)m}} - \frac{1}{2}\tilde{\Gamma}^m\partial_i\tilde{\gamma}_{jm} - \frac{1}{2}\tilde{\Gamma}^m\partial_j\tilde{\gamma}_{mi} + \frac{1}{2}\tilde{\Gamma}^r\partial_j\tilde{\gamma}_{ir} \\ & -\frac{1}{2}\partial_j\tilde{\gamma}^{kl}\partial_k\tilde{\gamma}_{li} + \frac{1}{2}\tilde{\Gamma}^r\partial_i\tilde{\gamma}_{jr} - \frac{1}{2}\partial_i\tilde{\gamma}^{kl}\partial_k\tilde{\gamma}_{lj} - \tilde{\gamma}^{mn}\tilde{\gamma}^{kl}\tilde{\Gamma}_{nik}\tilde{\Gamma}_{lmj}\end{aligned} \tag{G.87}$$

From Eq. (G.85), we conclude

$$\begin{aligned} & \tilde{\Gamma}_{lmj} + \tilde{\Gamma}_{mlj} = \partial_j\tilde{\gamma}_{lm} \\ \Rightarrow \quad & -\tilde{\gamma}^{mn}\tilde{\gamma}^{kl}\tilde{\Gamma}_{nik}\tilde{\Gamma}_{lmj} = \tilde{\gamma}^{mn}\tilde{\gamma}^{kl}\tilde{\Gamma}_{nik}(\tilde{\Gamma}_{mlj} - \partial_j\tilde{\gamma}_{lm}) = \tilde{\gamma}^{kl}\tilde{\Gamma}^m_{ik}\tilde{\Gamma}_{mlj} + \tilde{\Gamma}_{nik}\partial_j\tilde{\gamma}^{nk}\,,\end{aligned} \tag{G.88}$$

so that

$$\tilde{\mathcal{R}}_{ij} = -\frac{1}{2}\tilde{\gamma}^{km}\partial_k\partial_m\tilde{\gamma}_{ij} + \tilde{\gamma}_{m(i}\partial_{j)}\tilde{\Gamma}^m + \tilde{\Gamma}^m\tilde{\Gamma}_{(ij)m} - \frac{1}{2}\partial_j\tilde{\gamma}^{kl}\partial_k\tilde{\gamma}_{li} - \frac{1}{2}\partial_i\tilde{\gamma}^{kl}\partial_k\tilde{\gamma}_{lj} + \tilde{\gamma}^{kl}\tilde{\Gamma}^m_{ik}\tilde{\Gamma}_{mlj} + \tilde{\Gamma}_{nik}\partial_j\tilde{\gamma}^{nk}\,.$$

The 1st, 3rd and 4th term from the back still need some manipulation. We achieve this by considering

$$\begin{aligned}\tilde{\gamma}^{mn}\tilde{\Gamma}^k_{mi}\tilde{\Gamma}_{jkn} = {} & \frac{1}{4}\tilde{\gamma}^{mn}\tilde{\gamma}^{kr}\left(\partial_m\tilde{\gamma}_{ir} + \partial_i\tilde{\gamma}_{rm} - \partial_r\tilde{\gamma}_{mi}\right)\left(\partial_k\tilde{\gamma}_{nj} + \partial_n\tilde{\gamma}_{jk} - \partial_j\tilde{\gamma}_{kn}\right) \\ = {} & \frac{1}{4}\tilde{\gamma}^{mn}\tilde{\gamma}^{kr}\Big(\partial_r\tilde{\gamma}_{mi}\partial_j\tilde{\gamma}_{kn} - \partial_r\tilde{\gamma}_{mi}\partial_k\tilde{\gamma}_{nj} - \partial_r\tilde{\gamma}_{mi}\partial_n\tilde{\gamma}_{jk} - \partial_m\tilde{\gamma}_{ir}\partial_j\tilde{\gamma}_{kn} + \partial_m\tilde{\gamma}_{ir}\partial_k\tilde{\gamma}_{nj} \\ & + \partial_m\tilde{\gamma}_{ir}\partial_n\tilde{\gamma}_{jk} - \partial_i\tilde{\gamma}_{rm}\partial_j\tilde{\gamma}_{kn} + \partial_i\tilde{\gamma}_{rm}\partial_k\tilde{\gamma}_{nj} + \partial_i\tilde{\gamma}_{rm}\partial_n\tilde{\gamma}_{jk}\Big) \\ \Rightarrow 2\tilde{\gamma}^{mn}\tilde{\Gamma}^k_{m(i}\tilde{\Gamma}_{j)kn} = {} & \frac{1}{4}\tilde{\gamma}^{mn}\tilde{\gamma}^{kr}\Big(\partial_r\tilde{\gamma}_{mi}\partial_j\tilde{\gamma}_{kn} - \partial_m\tilde{\gamma}_{ir}\partial_j\tilde{\gamma}_{kn} - \partial_i\tilde{\gamma}_{rm}\partial_j\tilde{\gamma}_{kn} + \partial_i\tilde{\gamma}_{rm}\partial_k\tilde{\gamma}_{nj} + \partial_i\tilde{\gamma}_{rm}\partial_n\tilde{\gamma}_{jk} \\ & + \partial_r\tilde{\gamma}_{mj}\partial_i\tilde{\gamma}_{kn} - \partial_m\tilde{\gamma}_{jr}\partial_i\tilde{\gamma}_{kn} - \partial_j\tilde{\gamma}_{rm}\partial_i\tilde{\gamma}_{kn} + \partial_j\tilde{\gamma}_{rm}\partial_k\tilde{\gamma}_{ni} + \partial_j\tilde{\gamma}_{rm}\partial_n\tilde{\gamma}_{ik}\Big)\,,\end{aligned}$$

where both the dashed and dotted pairs cancel while the other pairs contain duplicate terms and thus lead to factors of 2. We compare this with

$$\tilde{\Gamma}_{nik}\partial_j\tilde{\gamma}^{nk} - \frac{1}{2}\partial_j\tilde{\gamma}^{kl}\partial_k\tilde{\gamma}_{il} - \frac{1}{2}\partial_i\tilde{\gamma}^{kl}\partial_k\tilde{\gamma}_{lj}$$

$$
\begin{aligned}
&= -\frac{1}{2}\Big(\underline{\underline{\partial_i\tilde\gamma_{kn}}}\underbrace{+\partial_k\tilde\gamma_{ni}-\partial_n\tilde\gamma_{ik}}_{\to 0}\Big)\tilde\gamma^{nr}\tilde\gamma^{ks}\partial_j\tilde\gamma_{rs}+\underline{\frac{1}{2}\tilde\gamma^{kr}\tilde\gamma^{ls}\partial_j\tilde\gamma_{rs}\partial_k\tilde\gamma_{il}}+\frac{1}{2}\tilde\gamma^{kr}\tilde\gamma^{ls}\partial_i\tilde\gamma_{rs}\partial_k\tilde\gamma_{lj} \\
&= 2\tilde\gamma^{mn}\tilde\Gamma^k_{m(i}\tilde\Gamma_{j)kn}\,, \qquad \text{(G.89)}
\end{aligned}
$$

where in the second line, we have marked the terms with the same linestyles as the non-vanishing pairs in the previous result. This allows us to replace the 1st, 3rd and 4th term in the above result for $\mathcal{R}_{ij}$,

$$
\tilde{\mathcal{R}}_{ij} = -\frac{1}{2}\tilde\gamma^{km}\partial_k\partial_m\tilde\gamma_{ij}+\tilde\gamma_{m(i}\partial_{j)}\tilde\Gamma^m+\tilde\Gamma^m\tilde\Gamma_{(ij)m}+\underbrace{\tilde\gamma^{kl}\tilde\Gamma^m_{ik}\tilde\Gamma_{mjl}}_{=\tilde\gamma^{mn}\tilde\Gamma^k_{im}\tilde\Gamma_{kjn}}+2\tilde\gamma^{mn}\tilde\Gamma^k_{m(i}\tilde\Gamma_{j)kn}\,. \qquad \text{(G.90)}
$$

Note that second derivatives of the metric $\tilde\gamma_{ij}$ now appear only in the first term and in the form of the spatial part of the wave operator. This rearrangement of second derivatives through the introduction of the auxiliary variable $\tilde\Gamma^i$ is an important ingredient for the success of the BSSNOK formulation.

Next, we consider the χ contribution to the Ricci tensor. We start with Eq. (G.80),

$$
\begin{aligned}
\mathcal{R}^\chi_{ij} &= -\partial_m f^m_{ij}+\partial_j f^m_{im}-\tilde\Gamma^n_{ij}f^m_{nm}+f^n_{ij}f^m_{nm}+f^n_{im}\tilde\Gamma^m_{nj}+\tilde\Gamma^n_{im}f^m_{nj}-f^n_{im}f^m_{nj}\,, \\
f^i_{jk} &= \frac{1}{2\chi}\left(\delta^i{}_k\partial_j\chi+\delta^i{}_j\partial_k\chi-\tilde\gamma_{jk}\tilde\gamma^{im}\partial_m\chi\right)\,, \\
\Rightarrow f^k_{jk} &= \frac{1}{2\chi}3\partial_j\chi = \frac{3}{2}\frac{\partial_j\chi}{\chi}\,.
\end{aligned}
$$

Plugging the f terms into $\mathcal{R}^\chi_{ij}$ gives a lengthy but straightforward expression,

$$
\begin{aligned}
\mathcal{R}^\chi_{ij} &= -\partial_m\left\{\frac{1}{2\chi}\left(\delta^m{}_j\partial_i\chi+\delta^m{}_i\partial_j\chi-\tilde\gamma_{ij}\tilde\gamma^{mn}\partial_n\chi\right)\right\}+\frac{3}{2}\partial_j\left\{\frac{\partial_i\chi}{\chi}\right\}-\tilde\Gamma^n_{ij}\frac{3}{2}\frac{\partial_n\chi}{\chi} \\
&\quad+\frac{1}{2\chi}\left(\delta^n{}_j\partial_i\chi+\delta^n{}_i\partial_j\chi-\tilde\gamma_{ij}\tilde\gamma^{mn}\partial_m\chi\right)\frac{3}{2}\frac{\partial_n\chi}{\chi}+\frac{1}{2\chi}\left(\delta^n{}_m\partial_i\chi+\delta^n{}_i\partial_m\chi-\tilde\gamma_{im}\tilde\gamma^{nk}\partial_k\chi\right)\tilde\Gamma^m_{nj} \\
&\quad+\tilde\Gamma^n_{im}\frac{1}{2\chi}\left(\delta^m{}_j\partial_n\chi+\delta^m{}_n\partial_j\chi-\tilde\gamma_{nj}\tilde\gamma^{mk}\partial_k\chi\right) \\
&\quad-\frac{1}{4\chi^2}\left(\delta^n{}_m\partial_i\chi+\delta^n{}_i\partial_m\chi-\tilde\gamma_{im}\tilde\gamma^{nk}\partial_k\chi\right)\left(\delta^m{}_j\partial_n\chi+\delta^m{}_n\partial_j\chi-\tilde\gamma_{nj}\tilde\gamma^{ml}\partial_l\chi\right) \\
&= \frac{1}{2\chi}\left(\underline{-\partial_j\partial_i\chi-\partial_i\partial_j\chi}+\partial_m\tilde\gamma_{ij}\tilde\gamma^{mn}\partial_n\chi+\tilde\gamma_{ij}\partial_m\tilde\gamma^{mn}\partial_n\chi+\tilde\gamma_{ij}\tilde\gamma^{mn}\partial_m\partial_n\chi\right) \\
&\quad+\frac{\partial_j\chi\partial_i\chi}{2\chi^2}+\frac{\partial_i\chi\partial_j\chi}{2\chi^2}-\tilde\gamma_{ij}\tilde\gamma^{mn}\frac{\partial_m\chi\partial_n\chi}{2\chi^2}+\underline{\frac{3}{2}\frac{\partial_j\partial_i\chi}{\chi}}-\frac{3}{2}\frac{\partial_j\chi\partial_i\chi}{\chi^2}-\underline{\underline{\frac{3}{2}\tilde\Gamma^n_{ij}\frac{\partial_n\chi}{\chi}}}
\end{aligned}
$$

$$
\begin{aligned}
&+\frac{3}{4\chi^2}\left\{\partial_j\chi\partial_i\chi+\partial_i\chi\partial_j\chi-\tilde{\gamma}_{ij}\tilde{\gamma}^{mn}\partial_m\chi\partial_n\chi\right\}+\frac{1}{2\chi}\underbrace{\tilde{\Gamma}^m_{mj}}_{=0}\partial_i\chi+\underline{\underline{\frac{1}{2\chi}\tilde{\Gamma}^m_{ij}\partial_m\chi}}-\frac{\tilde{\gamma}_{im}\tilde{\gamma}^{nk}}{2\chi}\tilde{\Gamma}^m_{nj}\partial_k\chi \\
&+\underline{\underline{\frac{1}{2\chi}\tilde{\Gamma}^n_{ij}\partial_n\chi}}+\underbrace{\tilde{\Gamma}^n_{in}}_{=0}\frac{1}{2\chi}\partial_j\chi-\frac{1}{2\chi}\tilde{\gamma}_{nj}\tilde{\gamma}^{mk}\tilde{\Gamma}^n_{im}\partial_k\chi-\frac{1}{4\chi^2}\Big\{\partial_i\chi\partial_j\chi+3\partial_i\chi\partial_j\chi-\partial_i\chi\partial_j\chi \\
&+\partial_i\chi\partial_j\chi+\partial_i\chi\partial_j\chi-\tilde{\gamma}_{ij}\tilde{\gamma}^{ml}\partial_m\chi\partial_l\chi-\tilde{\gamma}_{ij}\tilde{\gamma}^{nk}\partial_n\chi\partial_k\chi-\partial_i\chi\partial_j\chi+\partial_i\chi\partial_j\chi\Big\} \\
=\;&\frac{\partial_i\partial_j\chi}{\chi}\left\{-\frac{1}{2}-\frac{1}{2}+\frac{3}{2}\right\}+\frac{\partial_i\chi\partial_j\chi}{\chi^2}\left\{\frac{1}{2}+\frac{1}{2}-\frac{3}{2}+\frac{3}{2}-\frac{5}{4}\right\}+\frac{1}{\chi}\tilde{\gamma}_{ij}\tilde{\gamma}^{mn}\partial_m\partial_n\chi\left\{\frac{1}{2}\right\} \\
&+\frac{1}{\chi^2}\tilde{\gamma}_{ij}\tilde{\gamma}^{mn}\partial_m\chi\partial_n\chi\left\{-\frac{1}{2}-\frac{3}{4}+\frac{1}{2}\right\}+\frac{1}{2\chi}\partial_m\tilde{\gamma}_{ij}\tilde{\gamma}^{mn}\partial_n\chi+\frac{1}{2\chi}\tilde{\gamma}_{ij}\partial_m\tilde{\gamma}^{mn}\partial_n\chi \\
&+\frac{1}{\chi}\tilde{\Gamma}^m_{ij}\partial_m\chi\left\{-\frac{3}{2}+\frac{1}{2}+\frac{1}{2}\right\}+\frac{1}{2\chi}\left(-\tilde{\gamma}_{im}\tilde{\gamma}^{nk}\tilde{\Gamma}^m_{nj}\partial_k\chi-\tilde{\gamma}_{nj}\tilde{\gamma}^{mk}\tilde{\Gamma}^n_{im}\partial_k\chi\right) \\
=\;&\frac{\partial_i\partial_j\chi}{2\chi}-\frac{\partial_i\chi\partial_j\chi}{4\chi^2}+\frac{1}{2\chi}\tilde{\gamma}_{ij}\tilde{\gamma}^{mn}\partial_m\partial_n\chi-\frac{3}{4}\tilde{\gamma}_{ij}\tilde{\gamma}^{mn}\frac{\partial_m\chi\partial_n\chi}{\chi^2}+\frac{\partial_k\chi}{2\chi}\left(\underline{\partial_m\tilde{\gamma}_{ij}\tilde{\gamma}^{mk}+\tilde{\gamma}_{ij}\partial_m\tilde{\gamma}^{mk}}\right) \\
&-\frac{1}{2\chi}\tilde{\Gamma}^m_{ij}\partial_m\chi-\frac{1}{2\chi}\left(\underline{\tilde{\Gamma}_{inj}\tilde{\gamma}^{nk}+\tilde{\Gamma}_{jim}\tilde{\gamma}^{mk}}\right)\partial_k\chi\,. \qquad \text{(G.91)}
\end{aligned}
$$

The terms underlined in the last expression simplify according to

$$
\begin{aligned}
&\partial_m\tilde{\gamma}_{ij}\tilde{\gamma}^{mk}+\tilde{\gamma}_{ij}\partial_m\tilde{\gamma}^{mk}-\frac{1}{2}\Big(\partial_n\tilde{\gamma}_{ji}+\partial_j\tilde{\gamma}_{in}-\partial_i\tilde{\gamma}_{nj}\Big)\tilde{\gamma}^{nk}-\frac{1}{2}\Big(\partial_i\tilde{\gamma}_{mj}+\partial_m\tilde{\gamma}_{ji}-\partial_j\tilde{\gamma}_{im}\Big)\tilde{\gamma}^{mk} \\
=\;&\tilde{\gamma}_{ij}\partial_m\tilde{\gamma}^{mk}\,, \qquad \text{(G.92)}
\end{aligned}
$$

so that

$$
\mathcal{R}^{\chi}_{ij}=\frac{-1}{4\chi^2}\left(\partial_i\chi\partial_j\chi+3\tilde{\gamma}_{ij}\tilde{\gamma}^{mn}\partial_m\chi\partial_n\chi\right)+\frac{1}{2\chi}\Big(\underbrace{\partial_i\partial_j\chi-\tilde{\Gamma}^m_{ij}\partial_m\chi}_{=\tilde{D}_i\tilde{D}_j\chi}+\underline{\tilde{\gamma}_{ij}\tilde{\gamma}^{mn}\partial_m\partial_n\chi}+\underline{\tilde{\gamma}_{ij}\partial_m\tilde{\gamma}^{mk}\partial_k\chi}\Big)\,.
$$

Again, we have underlined terms which we can simplify, this time writing the trace of the second covariant derivative of χ as

$$
\begin{aligned}
\frac{1}{2\chi}\tilde{\gamma}_{ij}\tilde{\gamma}^{mn}\tilde{D}_m\tilde{D}_n\chi &= \frac{1}{2\chi}\tilde{\gamma}_{ij}\tilde{\gamma}^{mn}\left(\partial_m\partial_n\chi-\tilde{\Gamma}^l_{nm}\partial_l\chi\right) \\
&= \frac{1}{2\chi}\tilde{\gamma}_{ij}\tilde{\gamma}^{mn}\Big[\partial_m\partial_n\chi-\frac{1}{2}\tilde{\gamma}^{lk}\Big(\partial_n\tilde{\gamma}_{mk}+\partial_m\tilde{\gamma}_{kn}-\underbrace{\partial_k\tilde{\gamma}_{mn}}_{\to 0}\Big)\partial_l\chi\Big] \\
&= \frac{1}{2\chi}\left[\tilde{\gamma}_{ij}\tilde{\gamma}^{mn}\partial_m\partial_n\chi-\tilde{\gamma}_{ij}\tilde{\gamma}^{mn}\tilde{\gamma}^{lk}\partial_m\tilde{\gamma}_{nk}\partial_l\chi\right] \;=\; \frac{1}{2\chi}\left[\tilde{\gamma}_{ij}\tilde{\gamma}^{mn}\partial_m\partial_n\chi+\tilde{\gamma}_{ij}\partial_m\tilde{\gamma}^{ml}\partial_l\chi\right]\,,
\end{aligned}
$$

which gives the final version

$$\mathcal{R}^{\chi}_{ij} = \frac{-1}{4\chi^2}\left(\partial_i\chi\partial_j\chi + 3\tilde{\gamma}_{ij}\tilde{\gamma}^{mn}\partial_m\chi\partial_n\chi\right) + \frac{1}{2\chi}\left(\tilde{D}_i\tilde{D}_j\chi + \tilde{\gamma}_{ij}\tilde{\gamma}^{mn}\tilde{D}_m\tilde{D}_n\chi\right).$$

That leaves us with the second covariant derivative of the lapse which, fortunately, is much easier. We merely need Eq. (G.38) for the Christoffel symbols, whence

$$\begin{aligned} D_iD_j\alpha &= \partial_i\partial_j\alpha - \tilde{\Gamma}^m_{ji}\partial_m\alpha = \tilde{D}_i\tilde{D}_j\alpha + \frac{1}{2\chi}\left(\delta^m{}_i\partial_j\chi + \delta^m{}_j\partial_i\chi - \tilde{\gamma}_{ji}\tilde{\gamma}^{mn}\partial_n\chi\right)\partial_m\alpha \\ &= \tilde{D}_i\tilde{D}_j\alpha + \frac{1}{2\chi}\left(\partial_i\alpha\partial_j\chi + \partial_j\alpha\partial_i\chi - \tilde{\gamma}_{ij}\tilde{\gamma}^{mn}\partial_n\chi\partial_m\alpha\right) \\ &= \tilde{D}_i\tilde{D}_j\alpha + \frac{1}{\chi}\partial_{(i}\alpha\partial_{j)}\chi - \frac{1}{2\chi}\tilde{\gamma}_{ij}\tilde{\gamma}^{mn}\partial_m\chi\partial_n\alpha\,. \end{aligned} \tag{G.93}$$

□

With the BSSNOK system, we now have a viable set of PDEs that enables us to evolve the Einstein equations in time. But there remain two ingredients for a time evolution that we still need to address, initial data and how to specify the gauge variables α and β^i which, we recall, are not determined by the Einstein equations.

H Gauge and initial data

H.1 Initial data

As with so many other topic of our notes, we could again devote an entire lecture course to the construction of initial data. For the sake of brevity, our discussion will focus on the basic methodology and discuss the arguably most important case of black-hole binaries. Readers can find more details in Cook's Living Review article [42].

The calculation of initial data faces two main challenges, (i) solving the constraint equations and (ii) obtaining data that represent a snapshot of the physical system under consideration. For analytically known spacetimes, such as Schwarzschild or Kerr, obtaining initial data is straightforward. The evolution of these data also serves important purposes for code testing and calibration, but the central goal of numerical relativity is the simulation of spacetimes that cannot be modelled with analytical means. The calculation of initial data for such spacetimes often also involves numerical methods, but are still aided by analytic solutions which can be used to construct initial guesses for the elliptic solvers.

The constraint equations we aim to solve are the Hamiltonian and momentum constraints (F.96) and (F.97) which we repeat here for convenience,

$$\begin{aligned}
\mathcal{H} &= \mathcal{R} + K^2 - K_{mn}K^{mn} - 2\Lambda - 16\pi\rho\,, \\
\mathcal{M}_i &= D_i K - D_m K^m{}_i + 8\pi j_i = 0 \quad \Leftrightarrow \quad \mathcal{M}^i = D_m(\gamma^{mi}K - K^{mi}) + 8\pi j^i = 0\,.
\end{aligned}$$

In a sense that we will make clearer below, one often interprets the Hamiltonian constraint as one constraint on the spatial metric γ_{ij} and the momentum constraints as three constraints on the extrinsic curvature K_{ij}, leaving us with 5 independent components γ_{ij} and 3 K_{ij}. Given that GR has 2 degrees of freedom, we would only expect 2 independent components each for γ_{ij} and K_{ij}. This discrepancy is explained by the coordinate freedom of GR; lapse α and shift β^i determine how coordinates evolve in time, but we still have freedom in choosing the initial coordinates. Indeed, the spatial metric γ_{ij} is fully covariant in the three spatial dimensions, so that we have three spatial coordinates to specify on the initial hypersurface. Likewise, we determine the embedding of the initial hypersurface through specification of the time coordinate. Taking these into account, we end up with the expected two physical degrees of freedom for γ_{ij} and K_{ij}.

H.1.1 Conformal transformations

The central goal of this section is to formulate the constraints as an elliptic system of PDEs suitable for numerical algorithms. As it turns out, this is most conveniently achieved in terms of a conformal transformation similar, but not identical, to that we have encountered in our discussion of the BSSNOK formulation in Sec. G.3. In preparation for this calculation, we recapitulate the changes of the main curvature variables under conformal transformation.

Def. : Let $\mathcal{M}$ be an n-dimensional manifold with metric $\boldsymbol{\gamma}$. A conformal transformation of the metric is given by the multiplication with a scalar function,

$$\bar{\gamma}_{ij} = e^{2\varphi}\gamma_{ij} \qquad \Leftrightarrow \qquad \gamma_{ij} = e^{-2\varphi}\bar{\gamma}_{ij} \,. \tag{H.1}$$

Note that in this subsection, i and j run from 1 to n as we are discussing conformal transformations of metrics in n dimensions. Furthermore, we do not impose any condition on $\det \bar{\gamma}_{ij}$ here, unlike we did for the conformal metric in the BSSNOK formulation.

Proposition: The Christoffel symbols and curvature tensors associated with the two metrics $\bar{\gamma}_{ij} = e^{2\varphi}\gamma_{ij}$ in n dimensions are related by

$$\Gamma^i_{jk} = \bar{\Gamma}^i_{jk} - \Big(\delta^i{}_j\partial_k\varphi + \delta^i{}_k\partial_j\varphi - \underbrace{\bar{\gamma}_{jk}\bar{\gamma}^{im}}_{=\gamma_{jk}\gamma^{im}}\partial_m\varphi \,.\Big) \tag{H.2}$$

$$e^{2\varphi}\mathcal{R}_{ijkl} = \bar{\mathcal{R}}_{ijkl} + \bar{\gamma}_{ik}X_{jl} - \bar{\gamma}_{il}X_{jk} + \bar{\gamma}_{jl}X_{ik} - \bar{\gamma}_{jk}X_{il} \tag{H.3}$$

$$\begin{aligned} \text{with} \quad X_{jl} = X_{lj} &= \bar{D}_j\bar{D}_l\varphi + \partial_j\varphi\partial_l\varphi - \frac{1}{2}\bar{\gamma}_{jl}(\bar{\gamma}^{mn}\partial_m\varphi\partial_n\varphi) \\ &= D_jD_l\varphi - \partial_j\varphi\partial_l\varphi + \frac{1}{2}\bar{\gamma}_{jl}(\bar{\gamma}^{mn}\partial_m\varphi\partial_n\varphi) \end{aligned}$$

$$\begin{aligned} \mathcal{R}_{ij} &= \bar{\mathcal{R}}_{ij} + (n-2)\Big(\bar{D}_i\bar{D}_j\varphi + \partial_i\varphi\partial_j\varphi\Big) + \bar{\gamma}_{ij}\bar{\gamma}^{mn}\Big[\bar{D}_m\bar{D}_n\varphi - (n-2)\partial_m\varphi\partial_n\varphi\Big] \\ &= \bar{\mathcal{R}}_{ij} + (n-2)\Big(D_iD_j\varphi - \partial_i\varphi\partial_j\varphi\Big) + \gamma_{ij}\gamma^{mn}\Big[D_mD_n\varphi + (n-2)\partial_m\varphi\partial_n\varphi\Big] \,. \end{aligned} \tag{H.4}$$

$$\begin{aligned} \mathcal{R} &= e^{2\varphi}\Big\{\bar{\mathcal{R}} + (n-1)\bar{\gamma}^{mn}\Big[2\bar{D}_m\bar{D}_n\varphi - (n-2)\partial_m\varphi\partial_n\varphi\Big]\Big\} \\ &= e^{2\varphi}\bar{\mathcal{R}} + (n-1)\gamma^{mn}\left[2D_mD_n\varphi + (n-2)\partial_m\varphi\partial_n\varphi\right] \,. \end{aligned} \tag{H.5}$$

Proof. (1) We start with the Christoffel symbols,

$$\begin{aligned} \Gamma^i_{jk} &= \frac{1}{2}\gamma^{im}\left(\partial_j\gamma_{km} + \partial_k\gamma_{mj} - \partial_m\gamma_{jk}\right) \\ &= \frac{1}{2}e^{2\varphi}\bar{\gamma}^{im}\left[\partial_j\left(\bar{\gamma}_{km}e^{-2\varphi}\right) + \partial_k\left(\bar{\gamma}_{mj}e^{-2\varphi}\right) - \partial_m\left(\bar{\gamma}_{jk}e^{-2\varphi}\right)\right] \\ &= \bar{\Gamma}^i_{jk} - \Big(\delta^i{}_k\partial_j\varphi + \delta^i{}_j\partial_k\varphi - \bar{\gamma}_{jk}\bar{\gamma}^{im}\partial_m\varphi\Big) \end{aligned} \tag{H.6}$$

(2) The relation for the Riemann tensor is good deal harder to obtain. Writing

$$f^i_{jl} = \delta^i{}_j\partial_l\varphi + \delta^i{}_l\partial_j\varphi - \bar{\gamma}_{jl}\bar{\gamma}^{im}\partial_m\varphi \quad \Rightarrow \quad \Gamma^i_{jl} = \bar{\Gamma}^i_{jl} - f^i_{jl} \,, \tag{H.7}$$

$$\begin{aligned}
\Rightarrow\ \partial_k f^i_{jl} &= \delta^i{}_j \partial_k\partial_l\varphi + \delta^i{}_l \partial_k\partial_j\varphi - \bar\gamma_{jl}\bar\gamma^{im}\partial_k\partial_m\varphi - \partial_k\bar\gamma_{jl}\bar\gamma^{im}\partial_m\varphi - \bar\gamma_{jl}\partial_k\bar\gamma^{im}\partial_m\varphi \\
\wedge\ \ f^m_{jl} f^i_{mk} &= \Big\{\delta^m{}_j\partial_l\varphi + \delta^m{}_l\partial_j\varphi - \bar\gamma_{jl}\bar\gamma^{mn}\partial_n\varphi\Big\}\Big\{\delta^i{}_m\partial_k\varphi + \delta^i{}_k\partial_m\varphi - \bar\gamma_{mk}\bar\gamma^{ir}\partial_r\varphi\Big\}.
\end{aligned}$$

the Riemann tensor becomes

$$\begin{aligned}
\mathcal{R}^i{}_{jkl} &= \partial_k\Gamma^i_{jl} - \partial_l\Gamma^i_{jk} + \Gamma^m_{jl}\Gamma^i_{mk} - \Gamma^m_{jk}\Gamma^i_{ml} \\
&= \bar{\mathcal{R}}^i{}_{jkl} - \partial_k f^i_{jl} + \partial_l f^i_{jk} - \bar\Gamma^m_{jl} f^i_{mk} - f^m_{jl}\bar\Gamma^i_{mk} + f^m_{jl} f^i_{mk} + \bar\Gamma^m_{jk} f^i_{ml} + f^m_{jk}\bar\Gamma^i_{ml} - f^m_{jk} f^i_{ml} \\
&= \bar{\mathcal{R}}^i{}_{jkl} - \delta^i{}_j\partial_k\partial_l\varphi - \delta^i{}_l\partial_k\partial_j\varphi + \bar\gamma_{jl}\bar\gamma^{im}\partial_k\partial_m\varphi + \partial_k\bar\gamma_{jl}\bar\gamma^{im}\partial_m\varphi + \bar\gamma_{jl}\partial_k\bar\gamma^{im}\partial_m\varphi \\
&\quad \partial^i{}_j\partial_l\partial_k\varphi + \delta^i{}_k\partial_l\partial_j\varphi - \bar\gamma_{jk}\bar\gamma^{im}\partial_l\partial_m\varphi - \partial_l\bar\gamma_{jk}\bar\gamma^{im}\partial_m\varphi - \bar\gamma_{jk}\partial_l\bar\gamma^{im}\partial_m\varphi \\
&\quad -\bar\Gamma^m_{jl}(\delta^i{}_m\partial_k\varphi + \delta^i{}_k\partial_m\varphi - \bar\gamma_{mk}\bar\gamma^{in}\partial_n\varphi) + \bar\Gamma^m_{jk}(\delta^i{}_m\partial_l\varphi + \delta^i{}_l\partial_m\varphi - \bar\gamma_{ml}\bar\gamma^{in}\partial_n\varphi) \\
&\quad -\bar\Gamma^i_{mk}(\delta^m{}_j\partial_l\varphi + \delta^m{}_l\partial_j\varphi - \bar\gamma_{jl}\bar\gamma^{mn}\partial_n\varphi) + \bar\Gamma^i_{ml}(\delta^m{}_j\partial_k\varphi + \delta^m{}_k\partial_j\varphi - \bar\gamma_{jk}\bar\gamma^{mn}\partial_n\varphi) \\
&\quad +\Big\{\delta^i{}_j\partial_l\varphi\partial_k\varphi + \delta^i{}_k\partial_j\varphi\partial_l\varphi - \bar\gamma_{jk}\bar\gamma^{ir}\partial_r\varphi\partial_l\varphi + \delta^i{}_l\partial_j\varphi\partial_k\varphi + \delta^i{}_k\partial_j\varphi\partial_l\varphi \\
&\quad -\bar\gamma_{lk}\bar\gamma^{ir}\partial_j\varphi\partial_r\varphi - \bar\gamma_{jl}\bar\gamma^{in}\partial_k\varphi\partial_n\varphi - \delta^i{}_k\bar\gamma_{jl}\bar\gamma^{mn}\partial_n\varphi\partial_m\varphi + \bar\gamma_{jl}\bar\gamma^{ir}\partial_k\varphi\partial_r\varphi\Big\} \\
&\quad -\Big\{\delta^i{}_j\partial_k\varphi\partial_l\varphi + \delta^i{}_l\partial_j\varphi\partial_k\varphi - \bar\gamma_{jl}\bar\gamma^{ir}\partial_r\varphi\partial_k\varphi + \delta^i{}_k\partial_j\varphi\partial_l\varphi + \delta^i{}_l\partial_j\varphi\partial_k\varphi \\
&\quad -\bar\gamma_{kl}\bar\gamma^{ir}\partial_j\varphi\partial_r\varphi - \bar\gamma_{jk}\bar\gamma^{in}\partial_l\varphi\partial_n\varphi - \delta^i{}_l\bar\gamma_{jk}\bar\gamma^{mn}\partial_n\varphi\partial_m\varphi + \bar\gamma_{jk}\bar\gamma^{ir}\partial_l\varphi\partial_r\varphi\Big\} \\
&= -\delta^i{}_l\Big(\partial_k\partial_j\varphi - \bar\Gamma^m_{jk}\partial_m\varphi\Big) + \delta^i{}_k\Big(\partial_l\partial_j\varphi - \bar\Gamma^m_{jl}\partial_m\varphi\Big) + \bar\gamma_{jl}\bar\gamma^{im}\partial_k\partial_m\varphi \\
&\quad +\frac{1}{2}\bar\gamma^{ir}\Big(\partial_m\bar\gamma_{kr} + \partial_k\bar\gamma_{rm} - \partial_r\bar\gamma_{mk}\Big)\bar\gamma_{jl}\bar\gamma^{mn}\partial_n\varphi - \bar\gamma_{jl}\bar\gamma^{ir}\bar\gamma^{ms}\partial_k\bar\gamma_{rs}\partial_m\varphi \\
&\quad -\bar\gamma_{jk}\bar\gamma^{im}\partial_l\partial_m\varphi - \frac{1}{2}\bar\gamma^{ir}\Big(\partial_m\bar\gamma_{lr} + \partial_l\bar\gamma_{rm} - \partial_r\bar\gamma_{ml}\Big)\bar\gamma_{jk}\bar\gamma^{mn}\partial_n\varphi + \bar\gamma_{jk}\bar\gamma^{ir}\bar\gamma^{ms}\partial_l\bar\gamma_{rs}\partial_m\varphi \\
&\quad +\partial_k\bar\gamma_{jl}\bar\gamma^{im}\partial_m\varphi - \partial_l\bar\gamma_{jk}\bar\gamma^{im}\partial_m\varphi - \bar\Gamma^i_{jl}\partial_k\varphi + \bar\gamma_{mk}\bar\gamma^{in}\bar\Gamma^m_{jl}\partial_n\varphi + \bar\Gamma^i_{jk}\partial_l\varphi - \bar\gamma_{ml}\bar\gamma^{in}\partial_n\varphi\bar\Gamma^m_{jk} \\
&\quad -\bar\Gamma^i_{jk}\partial_l\varphi - \bar\Gamma^i_{lk}\partial_j\varphi + \bar\Gamma^i_{jl}\partial_k\varphi + \bar\Gamma^i_{kl}\partial_j\varphi - \bar\gamma_{jk}\bar\gamma^{ir}\partial_r\varphi\partial_l\varphi + \delta^i{}_k\partial_j\varphi\partial_l\varphi - \delta^i{}_k\bar\gamma_{jl}\bar\gamma^{mn}\partial_n\varphi\partial_m\varphi \\
&\quad +\bar\gamma_{jl}\bar\gamma^{ir}\partial_r\varphi\partial_k\varphi - \delta^i{}_l\partial_j\varphi\partial_k\varphi + \delta^i{}_l\bar\gamma_{jk}\bar\gamma^{mn}\partial_n\varphi\partial_m\varphi + \bar{\mathcal{R}}^i{}_{jkl} \\
&= -\delta^i{}_l\bar D_k\bar D_j\varphi + \delta^i{}_k\bar D_l\bar D_j\varphi + \bar\gamma_{jl}\bar\gamma^{im}\partial_k\partial_m\varphi - \frac{1}{2}\bar\gamma_{jl}\bar\gamma^{ir}\bar\gamma^{mn}\Big(-\partial_m\bar\gamma_{kr} + \partial_k\bar\gamma_{rm} + \partial_r\bar\gamma_{mk}\Big)\partial_n\varphi
\end{aligned}$$

$$
\begin{aligned}
& -\bar\gamma_{jk}\bar\gamma^{im}\partial_l\partial_m\varphi + \frac{1}{2}\bar\gamma_{jk}\bar\gamma^{ir}\bar\gamma^{mn}\Big(-\partial_m\bar\gamma_{lr} + \partial_l\bar\gamma_{rm} + \partial_r\bar\gamma_{ml}\Big)\partial_n\varphi + \bar\gamma^{im}\partial_k\bar\gamma_{jl}\partial_m\varphi \\
& -\bar\gamma^{im}\partial_l\bar\gamma_{jk}\partial_m\varphi + \bar\gamma_{mk}\bar\gamma^{in}\frac{1}{2}\bar\gamma^{mr}\Big(-\partial_r\bar\gamma_{jl} + \partial_j\bar\gamma_{lr} + \partial_l\bar\gamma_{rj}\Big)\partial_n\varphi \\
& -\bar\gamma_{ml}\bar\gamma^{in}\frac{1}{2}\bar\gamma^{mr}\Big(-\partial_r\bar\gamma_{jk} + \partial_j\bar\gamma_{kr} + \partial_k\bar\gamma_{rj}\Big)\partial_n\varphi - \bar\gamma_{jk}\bar\gamma^{ir}\partial_r\varphi\partial_l\varphi + \delta^i{}_k\partial_j\varphi\partial_l\varphi \\
& -\delta^i{}_k\bar\gamma_{jl}\bar\gamma^{mn}\partial_m\varphi\partial_n\varphi + \bar\gamma_{jl}\bar\gamma^{ir}\partial_r\varphi\partial_k\varphi - \delta^i{}_l\partial_j\varphi\partial_k\varphi + \delta^i{}_l\bar\gamma_{jk}\bar\gamma^{mn}\partial_n\varphi\partial_m\varphi + \bar{\mathcal{R}}^i{}_{jkl} \\
= \;& -\delta^i{}_l\bar D_k\bar D_j\varphi + \delta^i{}_k\bar D_l\bar D_j\varphi + \bar\gamma_{jl}\bar\gamma^{im}\partial_k\partial_m\varphi - \bar\gamma_{jl}\bar\gamma^{ir}\bar\Gamma^n_{kr}\partial_n\varphi - \bar\gamma_{jk}\bar\gamma^{im}\partial_l\partial_m\varphi + \bar\gamma_{jk}\bar\gamma^{ir}\bar\Gamma^n_{lr}\partial_n\varphi \\
& +\bar\gamma^{in}\partial_n\varphi\Big\{\underline{\partial_k\bar\gamma_{jl}-\partial_l\bar\gamma_{jk}}\underline{-\frac{1}{2}\partial_k\bar\gamma_{jl}} + \frac{1}{2}\partial_j\bar\gamma_{lk} + \underline{\frac{1}{2}\partial_l\bar\gamma_{kj}} + \underline{\frac{1}{2}\partial_l\bar\gamma_{jk}} - \frac{1}{2}\partial_j\bar\gamma_{kl}\underline{-\frac{1}{2}\partial_k\bar\gamma_{lj}}\Big\} \\
& -\bar\gamma_{jk}\bar\gamma^{im}\partial_m\varphi\partial_l\varphi + \delta^i{}_k\partial_j\varphi\partial_l\varphi + \bar\gamma_{jl}\bar\gamma^{im}\partial_m\varphi\partial_k\varphi - \delta^i{}_l\partial_j\varphi\partial_k\varphi - \delta^i{}_k\bar\gamma_{jl}\bar\gamma^{mn}\partial_m\varphi\partial_n\varphi \\
& +\delta^i{}_l\bar\gamma_{jk}\bar\gamma^{mn}\partial_n\varphi\partial_m\varphi + \bar{\mathcal{R}}^i{}_{jkl}
\end{aligned}
$$

$$
\begin{aligned}
\Rightarrow\; \mathcal{R}_{ijkl}e^{2\varphi} = \;& -\bar\gamma_{il}\bar D_k\bar D_j\varphi + \bar\gamma_{ik}\bar D_l\bar D_j\varphi + \bar\gamma_{jl}\delta_i{}^m\bar D_k\bar D_m\varphi - \bar\gamma_{jk}\delta_i{}^m\bar D_l\bar D_m\varphi \\
& -\bar\gamma_{jk}\partial_i\varphi\partial_l\varphi + \bar\gamma_{ik}\partial_j\varphi\partial_l\varphi + \bar\gamma_{jl}\partial_i\varphi\partial_k\varphi - \bar\gamma_{il}\partial_j\varphi\partial_k\varphi \\
& -\bar\gamma_{ik}\bar\gamma_{jl}\Big(\bar\gamma^{mn}\partial_m\varphi\partial_n\varphi\Big) + \bar\gamma_{il}\bar\gamma_{jk}\Big(\bar\gamma^{mn}\partial_n\varphi\partial_m\varphi\Big) + \bar{\mathcal{R}}_{ijkl} \\
= \;& -\bar\gamma_{il}\left[\bar D_k\bar D_j\varphi + \partial_k\varphi\partial_j\varphi - \frac{1}{2}\bar\gamma_{jk}\Big(\bar\gamma^{mn}\partial_m\varphi\partial_n\varphi\Big)\right] \\
& +\bar\gamma_{ik}\left[\bar D_l\bar D_j\varphi + \partial_l\varphi\partial_j\varphi - \frac{1}{2}\bar\gamma_{jl}\Big(\bar\gamma^{mn}\partial_m\varphi\partial_n\varphi\Big)\right] \\
& +\bar\gamma_{jl}\left[\bar D_k\bar D_i\varphi + \partial_k\varphi\partial_i\varphi - \frac{1}{2}\bar\gamma_{ik}\Big(\bar\gamma^{mn}\partial_m\varphi\partial_n\varphi\Big)\right] \\
& -\bar\gamma_{jk}\left[\bar D_l\bar D_i\varphi + \partial_l\varphi\partial_i\varphi - \frac{1}{2}\bar\gamma_{il}\Big(\bar\gamma^{mn}\partial_m\varphi\partial_n\varphi\Big)\right] \\
= \;& \mathcal{R}_{ijkl} + \bar\gamma_{ik}X_{jl} - \bar\gamma_{il}X_{jk} + \bar\gamma_{jl}X_{ik} - \bar\gamma_{jk}X_{il} \\
& \text{with}\quad X_{jl} = \bar D_j\bar D_l\varphi + \partial_j\varphi\partial_l\varphi - \frac{1}{2}\bar\gamma_{jl}\Big(\bar\gamma^{mn}\partial_m\varphi\partial_n\varphi\Big)\,.
\end{aligned}
$$

Finally,

$$
\begin{aligned}
\bar D_j\bar D_l\varphi &= \partial_j\partial_l\varphi - \bar\Gamma^m_{lj}\partial_m\varphi \;=\; \partial_j\partial_l\varphi - \Gamma^m_{lj}\partial_m\varphi - f^m_{lj}\partial_m\varphi \\
&= D_jD_l\varphi - \partial_m\varphi\left(\delta^m{}_l\partial_j\varphi + \delta^m{}_j\partial_l\varphi - \bar\gamma_{jl}\bar\gamma^{mn}\partial_n\varphi\right)
\end{aligned}
$$

$$= \quad D_j D_l\varphi - 2\partial_j\varphi\partial_l\varphi + \bar{\gamma}_{jl}\bar{\gamma}^{mn}\partial_m\varphi\partial_n\varphi\,, \tag{H.8}$$

so that

$$X_{jl} = D_j D_l\varphi - \partial_j\varphi\partial_l\varphi + \frac{1}{2}\bar{\gamma}_{jl}\bar{\gamma}^{mn}\partial_m\varphi\partial_n\varphi \tag{H.9}$$

(3) We write the Ricci tensor as

$$\begin{aligned}
\mathcal{R}_{ij} &= \gamma^{mn}\mathcal{R}_{minj} = \bar{\gamma}^{mn}e^{2\varphi}\mathcal{R}_{ijkl} \\
&= \bar{\mathcal{R}}_{ij} + \bar{\gamma}^{mn}\left(\bar{\gamma}_{mn}X_{ij} - \bar{\gamma}_{mj}X_{im} + \bar{\gamma}_{ij}X_{mn} - \bar{\gamma}_{in}X_{mj}\right) \\
&= \bar{\mathcal{R}}_{ij} + (n-2)X_{ij} + \bar{\gamma}_{ij}\bar{\gamma}^{mn}X_{mn}\,.
\end{aligned}$$

Using $X_{mn} = \bar{D}_m\bar{D}_n + \partial_m\varphi\partial_n\varphi - \bar{\gamma}_{mn}(\bar{\gamma}^{rs}\partial_r\varphi\partial_s\varphi)/2$, we obtain

$$\bar{\gamma}^{mn}X_{mn} = \bar{D}^m\bar{D}_m\varphi + \frac{2-n}{2}\bar{\gamma}^{mn}\partial_m\varphi\partial_n\varphi\,,$$

and therefore

$$\begin{aligned}
\mathcal{R}_{ij} &= \bar{\mathcal{R}}_{ij} + (n-2)\left[\bar{D}_i\bar{D}_j\varphi + \partial_i\varphi\partial_j\varphi - \frac{1}{2}\bar{\gamma}_{ij}\bar{\gamma}^{mn}\partial_m\varphi\partial_n\varphi\right] + \bar{\gamma}_{ij}\left[\bar{D}^m\bar{D}_m\varphi - \frac{n-2}{2}\bar{\gamma}^{mn}\partial_m\varphi\partial_n\varphi\right] \\
&= \bar{\mathcal{R}}_{ij} + (n-2)\Big(\bar{D}_i\bar{D}_j\varphi + \partial_i\varphi\partial_j\varphi\Big) + \bar{\gamma}_{ij}\bar{D}^m\bar{D}_m\varphi - (n-2)\bar{\gamma}_{ij}\bar{\gamma}^{mn}\partial_m\varphi\partial_n\varphi\,.
\end{aligned}$$

In order to express the differences in terms of the original metric γ_{ij}, we use Eq. (H.8),

$$\begin{aligned}
\mathcal{R}_{ij} &= \bar{\mathcal{R}}_{ij} + (n-2)\Big(D_iD_j\varphi - 2\partial_i\varphi\partial_j\varphi + \underline{\gamma_{ij}\gamma^{mn}\partial_m\varphi\partial_n\varphi} + \partial_i\varphi\partial_j\varphi\Big) \\
&\quad + \gamma_{ij}\gamma^{mn}\left(D_mD_n\varphi - 2\partial_m\varphi\partial_n\varphi + \gamma_{mn}\gamma^{rs}\partial_r\varphi\partial_s\varphi\right)\underline{-(n-2)\gamma_{ij}\gamma^{mn}\partial_m\varphi\partial_n\varphi} \\
&= \bar{\mathcal{R}}_{ij} + (n-2)\Big(D_iD_j\varphi - \partial_i\varphi\partial_j\varphi\Big) + \gamma_{ij}\gamma^{mn}\Big[D_mD_n\varphi + (n-2)\partial_m\varphi\partial_n\varphi\Big]\,.
\end{aligned} \tag{H.10}$$

(4) The transformation of the Ricci scalar is obtained from

$$\begin{aligned}
\mathcal{R} &= e^{2\varphi}\bar{\gamma}^{mn}\mathcal{R}_{mn} \\
&= e^{2\varphi}\Big\{\bar{\mathcal{R}} + (n-2)\bar{D}^m\bar{D}_m\varphi + (n-2)\bar{\gamma}^{mn}\partial_m\varphi\partial_n\varphi + n\bar{D}^m\bar{D}_m\varphi - n(n-2)\bar{\gamma}^{mn}\partial_m\varphi\partial_n\varphi\Big\} \\
&= e^{2\varphi}\Big\{\bar{\mathcal{R}} + (2n-2)\bar{D}^m\bar{D}_m\varphi - (n-1)(n-2)\bar{\gamma}^{mn}\partial_m\varphi\partial_n\varphi\Big\}
\end{aligned} \tag{H.11}$$

Likewise, contracting Eq. (H.10) with γ^{ij} gives us

$$\begin{aligned}
\mathcal{R} &= e^{2\varphi}\bar{\mathcal{R}} + (n-2)D^mD_m\varphi - (n-2)\gamma^{mn}\partial_m\partial_n\varphi + n\gamma^{mn}\left[D_mD_n\varphi + (n-2)\partial_m\varphi\partial_n\varphi\right] \\
&= e^{2\varphi}\bar{\mathcal{R}} + 2(n-1)\gamma^{mn}D_mD_n\varphi + (n-2)(n-1)\gamma^{mn}\partial_m\varphi\partial_n\varphi\,.
\end{aligned} \tag{H.12}$$

□

H.1.2 The York-Lichnerowicz conformal traceless split

It is customary in the initial data literature to write the conformal factor as ψ^4 instead of the exponential $e^{2\varphi}$ we have used above and which enabled us to bypass some handling of tensor densities in the derivation of the curvature tensors. The conversion to ψ^4 is straightforward, though, now that we have obtained the conformal relations. It furthermore turns out convenient to separate the trace from the extrinsic curvature and conformally rescale the traceless part. The conformal decomposition of the spatial metric dates back to Lichnerowicz's work [43] whereas the split of the extrinsic curvature was developed some decades later by York [44, 45]. The variables thus obtained are summarized as follows.

Def. : The conformal traceless decomposition of the constraint equations employs the variables

$$\gamma_{ij} = \psi^4 \bar{\gamma}_{ij} = e^{-2\varphi} \bar{\gamma}_{ij} \qquad \Leftrightarrow \qquad \gamma^{ij} = \psi^{-4} \bar{\gamma}^{ij} = e^{2\varphi} \bar{\gamma}^{ij} \,, \tag{H.13}$$

$$K_{ij} = A_{ij} + \frac{1}{3} \gamma_{ij} K \,, \tag{H.14}$$

$$A_{ij} = \psi^{-2} \bar{A}_{ij} \qquad \Leftrightarrow \qquad A^{ij} = \psi^{-10} \bar{A}^{ij} \,. \tag{H.15}$$

Here ψ is a free function. Note that we do *not* require $\det \bar{\gamma}_{ij} = 1$ at this point.

Note the different conformal factor in the rescaling of A_{ij} compared to that used for the BSSNOK variables in Eq. (G.36). The specific choice of ψ^{-2} leads to some convenient cancellation of terms in our calculations; the factor ψ^{-10} for $\bar{A}^{ij}$ follows from raising the indices with $\bar{\gamma}^{ij}$.

Lemma: For the conformal transformation (H.13), the Christoffel symbols and Ricci scalar transform according to

$$\Gamma^i_{jk} = \bar{\Gamma}^i_{jk} + \frac{2}{\psi} \left(\delta^i{}_j \partial_k \psi + \delta^i{}_k \partial_j \psi - \bar{\gamma}_{jk} \bar{\gamma}^{im} \partial_m \psi \right) \,, \tag{H.16}$$

$$\mathcal{R} = \psi^{-4} \bar{\mathcal{R}} - \frac{8}{\psi^5} \bar{\gamma}^{mn} \bar{D}_m \bar{D}_n \psi \,. \tag{H.17}$$

Proof. Comparing the conformal transformations (H.1) and (H.13). we find

$$e^{-2\varphi} = \psi^4 \qquad \Rightarrow \qquad \varphi = -2 \ln \psi \qquad \Rightarrow \qquad \partial \varphi = -2 \frac{\partial \psi}{\psi}$$

$$\Rightarrow \quad \bar{D}_m \bar{D}_n \varphi = \bar{D}_m \left(-2 \frac{\bar{D}_n \psi}{\psi} \right) = -\frac{2}{\psi} \bar{D}_m \bar{D}_n \psi + \frac{2}{\psi^2} \partial_n \psi \partial_m \psi \,.$$

Inserting these into Eq. (H.2), we obtain

$$
\begin{aligned}
\Gamma^i_{jk} &= \bar{\Gamma}^i_{jk} - \left(\delta^i{}_j \partial_k \varphi + \delta^i{}_k \partial_j \varphi - \bar{\gamma}_{jk} \bar{\gamma}^{im} \partial_m \varphi\right) \\
&= \bar{\Gamma}^i_{jk} + \frac{2}{\psi} \left(\delta^i{}_j \partial_k \psi + \delta^i{}_k \partial_j \psi - \bar{\gamma}_{jk} \bar{\gamma}^{im} \partial_m \psi\right) , \qquad \text{(H.18)}
\end{aligned}
$$

and inserting them into Eq. (H.5) with $n = 3$, we get

$$
\begin{aligned}
\mathcal{R} &= \psi^{-4} \left[\bar{\mathcal{R}} + 2\bar{\gamma}^{mn} \left(-\frac{4}{\psi} \bar{D}_m \bar{D}_n \psi + \frac{4}{\psi^2} \partial_n \psi \partial_m \psi - \frac{4}{\psi^2} \partial_m \psi \partial_n \psi\right)\right] \\
&= \psi^{-4} \bar{\mathcal{R}} - \frac{8}{\psi^5} \bar{\gamma}^{mn} \bar{D}_m \bar{D}_n \psi \, . \qquad \text{(H.19)}
\end{aligned}
$$

□

Proposition: In terms of the conformal variables defined in Eqs. (H.13)-(H.15) the constraint equations become

$$
\bar{\mathcal{H}} := 8\bar{\gamma}^{mn} \bar{D}_m \bar{D}_n \psi - \psi \bar{\mathcal{R}} - \frac{2}{3} \psi^5 K^2 + \psi^{-7} \bar{A}_{mn} \bar{A}^{mn} + 2\psi^5 \Lambda + 16\pi \psi^5 \rho = 0 \qquad \text{(H.20)}
$$

$$
\bar{\mathcal{M}}^i := \bar{D}_m \bar{A}^{mi} - \frac{2}{3} \psi^6 \bar{\gamma}^{mi} \partial_m K - 8\pi \psi^{10} j^i = 0 \, . \qquad \text{(H.21)}
$$

Proof. With Eq. (H.17), the Hamiltonian constraint (F.96) becomes

$$
\mathcal{H} = \psi^{-4} \bar{\mathcal{R}} - \frac{8}{\psi^5} \bar{\gamma}^{mn} \bar{D}_m \bar{D}_n \psi + K^2 - K_{mn} K^{mn} - 2\Lambda - 16\pi \rho = 0 \, . \qquad \text{(H.22)}
$$

The definitions (H.14) and (H.15) imply

$$
K^2 - K_{mn} K^{mn} = K^2 - \left(A_{mn} + \frac{1}{3} \gamma_{mn} K\right) \left(A^{mn} + \frac{1}{3} \gamma^{mn} K\right) = K^2 - A_{mn} A^{mn} - \frac{1}{3} K^2 = \frac{2}{3} K^2 - A_{mn} A^{mn} \, ,
$$

so that

$$
8\bar{\gamma}^{mn} \bar{D}_m \bar{D}_n \psi - \psi \bar{\mathcal{R}} - \frac{2}{3} \psi^5 K^2 + \psi^5 \underbrace{A_{mn} A^{mn}}_{= \psi^{-12} \bar{A}_{mn} \bar{A}^{mn}} + 2\psi^5 \Lambda + 16\pi \psi^5 \rho = 0 \, . \qquad \text{(H.23)}
$$

The momentum constraint (F.97) can be written as

$$
\mathcal{M}^i = D_m \left(\gamma^{im} K - K^{im}\right) + 8\pi j^i = 0 \, .
$$

With the definition (H.14), we find

$$D_m(\gamma^{mi}K-K^{mi}) = D_m\left(\gamma^{mi}K - A^{mi} - \frac{1}{3}\gamma^{mi}K\right) = D_m\left(\frac{2}{3}\gamma^{mi}K - A^{mi}\right) = \frac{2}{3}\gamma^{mi}D_mK - D_mA^{mi}\,. \tag{H.24}$$

With the Christoffel symbols (H.16), the last term becomes

$$\begin{aligned}
D_mA^{mi} &= \partial_m\left(\psi^{-10}\bar{A}^{mi}\right) + \Gamma^m_{rm}\bar{A}^{ri}\psi^{-10} + \Gamma^i_{rm}\bar{A}^{mr}\psi^{-10} \\
&= \psi^{-10}\partial_m\bar{A}^{mi} - 10\bar{A}^{mi}\psi^{-11}\partial_m\psi + \bar{\Gamma}^m_{rm}\bar{A}^{ri}\psi^{-10} + \bar{\Gamma}^i_{rm}\bar{A}^{mr}\psi^{-10} \\
&\quad + \frac{2}{\psi^{11}}\left(\delta^m{}_r\partial_m\psi + \delta^m{}_m\partial_r\psi - \bar{\gamma}_{rm}\bar{\gamma}^{mn}\partial_n\psi\right)\bar{A}^{ri} + \frac{2}{\psi^{11}}\left(\delta^i{}_r\partial_m\psi + \delta^i{}_m\partial_r\psi - \bar{\gamma}_{rm}\bar{\gamma}^{ik}\partial_k\psi\right)\bar{A}^{mr} \\
&= \psi^{-10}\bar{D}_m\bar{A}^{mi} - 10\psi^{-11}\bar{A}^{mi}\partial_m\psi + \frac{2}{\psi^{11}}\left[\bar{A}^{mi}\partial_m\psi + 3\bar{A}^{ri}\partial_r\psi - \bar{A}^{ni}\partial_n\psi + \bar{A}^{mi}\partial_m\psi + \bar{A}^{ri}\partial_r\psi - 0\right] \\
&= \psi^{-10}\bar{D}_m\bar{A}^{mi}\,.
\end{aligned}$$

The cancellation of the $\partial_m\psi$ terms in the last step is the simplifying benefit of the choice of the exponent ψ^{-2} in the definition (H.15). The momentum constraint then becomes

$$\begin{aligned}
\mathcal{M}^i &= \frac{2}{3}\gamma^{mi}\partial_mK - \psi^{-10}\bar{D}_m\bar{A}^{mi} + 8\pi j^i = \frac{2}{3}\psi^{-4}\bar{\gamma}^{mi}\partial_mK - \psi^{-10}\bar{D}_m\bar{A}^{mi} + 8\pi j^i \\
\Rightarrow\ \bar{\mathcal{M}}^i &= \bar{D}_m\bar{A}^{mi} - \frac{2}{3}\psi^6\bar{\gamma}^{mi}\partial_mK - 8\pi\psi^{10}j^i = 0\,.
\end{aligned}$$

□

The key benefit of this reformulation of the constraints in terms of conformal variables arises from the following result which we quote without proof.

Proposition: Let $\bar{A}^{ij}$ be a symmetric and traceless tensor. There then exists a transverse, traceless symmetric tensor Q^{ij} (i.e. $\bar{D}_mQ^{mi}=0$ and $Q^m{}_m=0$) and a vector field X^i such that

$$\bar{A}^{ij} = Q^{ij} + (\mathbb{L}X)^{ij} := Q^{ij} + \bar{D}^iX^j + \bar{D}^jX^i - \frac{2}{3}\bar{\gamma}^{ij}\bar{D}_mX^m\,. \tag{H.25}$$

Note that $(\mathbb{L}X)^{ij}$ is traceless by construction, $(\mathbb{L}X)_m{}^m = 0$.

We have named the symmetric traceless tensor $\bar{A}^{ij}$ here since we are interested in Eq. (H.25) applied to our conformal traceless extrinsic curvature, but the decomposition works just the same for any other symmetric traceless tensor S^{ij} and for any other metric g_{ij}. Crucially, Eq. (H.25) enables us to isolate the longitudinal part $(\mathbb{L}X)^{ij}$ and express it in terms of the vector potential X^i.

Proposition: The constraint equations in the conformal traceless decomposition are

$$\bar{\mathcal{H}} = 8\bar{\gamma}^{mn}\bar{D}_m\bar{D}_n\psi - \psi\bar{\mathcal{R}} - \frac{2}{3}\psi^5K^2 + \psi^{-7}\bar{A}_{mn}\bar{A}^{mn} + 2\psi^5\Lambda + 16\pi\psi^5\rho = 0\,, \tag{H.26}$$

$$\bar{\mathcal{M}}^i = \bar{D}^m\bar{D}_mX^i + \frac{1}{3}\bar{D}^i\bar{D}_mX^m + \bar{\mathcal{R}}^i{}_mX^m - \frac{2}{3}\psi^6\bar{\gamma}^{mi}\partial_mK - 8\pi\psi^{10}j^i = 0\,. \tag{H.27}$$

Proof. The Hamiltonian constraint is the same as in Eq. (H.20), so we only need to consider the momentum constraint (H.21). Inserting the right-hand side of Eq. (H.25) for $\bar{A}^{mi}$, we get

$$\begin{aligned}
\bar{D}_m\bar{A}^{mi} &= \bar{D}_mQ^{mi} + \bar{D}_m(\mathbb{L}X)^{mi} = \bar{D}_m(\mathbb{L}X)^{mi} = \bar{D}_m\left(\bar{D}^mX^i + \bar{D}^iX^m - \frac{2}{3}\bar{\gamma}^{mi}\bar{D}_nX^n\right) \\
&= \bar{D}_m\bar{D}^mX^i + \bar{D}_m\bar{D}^iX^m - \frac{2}{3}\bar{\gamma}^{mi}\bar{D}_m\bar{D}_nX^n \\
&= \bar{D}_m\bar{D}^mX^i + \bar{\gamma}^{in}\bar{D}_m\bar{D}_nX^m - \frac{2}{3}\bar{\gamma}^{in}\bar{D}_n\bar{D}_mX^m\,.
\end{aligned} \tag{H.28}$$

Next, we recall the Ricci identity, applied here for the conformal metric $\bar{\gamma}_{ij}$,

$$\begin{aligned}
&(\bar{D}_m\bar{D}_n - \bar{D}_n\bar{D}_m)X^k = \bar{\mathcal{R}}^k{}_{lmn}X^l \\
\Rightarrow\quad &\bar{D}_m\bar{D}_nX^m = \bar{D}_n\bar{D}_mX^m + \bar{\mathcal{R}}^m{}_{lmn}X^l = \bar{D}_n\bar{D}_mX^m + \bar{\mathcal{R}}_{ln}X^l \\
\Rightarrow\quad &\bar{D}_m\bar{A}^{mi} = \bar{D}_m\bar{D}^mX^i + \frac{1}{3}\bar{\gamma}^{in}\bar{D}_n\bar{D}_mX^m + \bar{\mathcal{R}}^i{}_mX^m\,.
\end{aligned}$$

Substituting this expression in the momentum constraint (H.21) gives us

$$\bar{D}^m\bar{D}_mX^i + \frac{1}{3}\bar{\gamma}^{in}\bar{D}_n\bar{D}_mX^m + \bar{\mathcal{R}}^i{}_mX^m - \frac{2}{3}\psi^6\bar{\gamma}^{mi}\partial_mK - 8\pi\psi^{10}j^i = 0\,.$$

□

In the asymptotically flat vacuum case, $\rho = j^i = \Lambda = 0$, we can summarize the benefit of our rearrangement of the constraint equations as follows.

(1) We can freely specify

- 5 free functions for the conformal metric $\bar{\gamma}_{ij}$,
- 1 function for the mean curvature K,
- 2 free functions for the transverse traceless part Q^{ij} of the extrinsic curvature.

(2) We then solve

- the Hamiltonian constraint (H.26) for the conformal factor ψ,

- the momentum constraint (H.27) for the three components of the vector potential X^i.

The benefit of this procedure is best illustrated with some examples. From this point on, we assume asymptotic flatness and set $\Lambda = 0$.

Examples

(1) Spatial slices where $K = 0$ are often referred to as maximal slices since their three-dimensional proper volume is maximized relative to other slices where $K \neq 0$. In this case the constraints decouple and can be solved separately. More specifically, (H.27) does not involve the conformal factor ψ and can therefore be solved on its own to determine X^i. Note that the momentum constraint is linear in X^i which allows us to superpose individual solutions to obtain new solutions. Once X^i is determined, it is inserted into the Hamiltonian constraint (H.26) which becomes a single PDE for the conformal factor ψ.

(2) In the case of vacuum ($\rho = 0 = j^i$), time symmetry ($K_{ij} = 0$) and conformal flatness, $\bar{\gamma}_{ij} = \delta_{ij}$, the Hamiltonian constraint simplifies to

$$\delta^{mn}\partial_m\partial_n\psi = 0\,, \tag{H.29}$$

and the momentum constraint in its original form (F.97) vanishes completely. In that case, we merely have to solve the flat-space Laplace equation for the conformal factor which is solved, for example, by

$$\psi = \frac{A}{r} + B\,, \tag{H.30}$$

with $r = \sqrt{x^2 + y^2 + z^2}$ and constants A, $B \in \mathbb{R}$. Strictly speaking, $\triangle\frac{1}{r} = -4\pi\delta(r)$, which is the solution of a point charge. In the case of black holes, the Einstein equations become irregular at the singularity and when we refer to black holes as vacuum solutions of the Einstein equations we are implicitly excluding singularities. The point $r = 0$ we cut out from the domain for this purpose is commonly referred to as a *puncture*[13]. With appropriate rescaling of the coordinates, we can set $A = \frac{M}{2}$, $B = 1$, so that

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

which is initial data for a Schwarzschild black hole in isotropic coordinates,

$$\begin{aligned} \mathrm{d}s^2 &= -\left(\frac{1-\frac{M}{2r}}{1+\frac{M}{2r}}\right)^2 \mathrm{d}t^2 + \left(1+\frac{M}{2r}\right)^4 (\mathrm{d}r^2 + r^2\mathrm{d}\theta^2 + r^2\sin^2\theta\mathrm{d}\phi^2) \\ &= -\left(\frac{1-\frac{M}{2r}}{1+\frac{M}{2r}}\right)^2 \mathrm{d}t^2 + \left(1+\frac{M}{2r}\right)^4 (\mathrm{d}x^2 + \mathrm{d}y^2 + \mathrm{d}z^2)\,. \end{aligned} \tag{H.31}$$

[13] In this case, the point $r = 0$ is a coordinate singularity and actually represents an asymptotically flat spatial infinity compressed into a single point.

Of course, evolving these initial data in time will simply reproduce the analytically known Schwarzschild solution which can be valuable for code testing but does not provide us with new physical insight. The linear character of the Laplace equation (H.29), however, allows us to superpose multiple solutions of the form (H.31) centered at spatial points $x^i_{(1)}$, $x^i_{(2)}$ etc. In this case, the conformal factor is given by

$$\psi = 1 + \sum_{i=1}^{n} \frac{M_{(i)}}{2|\boldsymbol{r} - \boldsymbol{r}_{(i)}|}\,, \tag{H.32}$$

which gives us initial data for n BHs with masses $M_{(1)}$, $M_{(2)}$, ... initially at rest at locations $\boldsymbol{x}_{(1)}$, $\boldsymbol{x}_{(2)}$ etc. These data are known as Brill-Lindquist data [46] and are still available in closed analytic form. For $n > 1$, however, the time evolution of these data is *not* known analytically and can only be obtained using numerical simulations. For the case $n = 2$, for example, Brill-Lindquist data represent two BHs some distance d apart and initially at rest. Evolved in time, they will collide head-on, merge into one single BH and emit GWs in the process. In fact, this emission of GW carries away some energy from the binary, so that the final BH has a mass a bit below $M_{(1)} + M_{(2)}$ [47].

H.1.3 Bowen-York and puncture data

Brill-Lindquist data is still rather limited since it only gives us initial data for non-spinning (Schwarzschild) BHs at rest. A slight generalization of our specified variables, however, turns out to overcome these restrictions. We still consider vacuum and conformally flat initial data but instead of requiring full time symmetry $K_{ij} = 0$, only impose the vanishing of the mean curvature $K = 0$ and the transverse part $Q^{ij} = 0$. But we allow for a non-zero longitudinal traceless contribution

$$\bar{A}^{ij} = \bar{D}^i X^j + \bar{D}^j X^i - \frac{2}{3}\bar{\gamma}^{ij}\bar{D}_m X^m \tag{H.33}$$

to the extrinsic curvature. This case leads to the so-called *Bowen-York data* [48] for the traceless extrinsic curvature and initial data for general BH binaries commonly referred to as *puncture data* [49]. We will discuss this case in more detail in the remainder of this section. For the case of Bowen-York data, i.e. $\bar{\gamma}_{ij} = \delta_{ij}$, $Q^{ij} = 0$ and $K = 0$ in vacuum, the momentum constraint (H.27) becomes

$$\bar{\mathcal{M}}^i = \partial^m\partial_m X^i + \frac{1}{3}\partial^i\partial_m X^m = 0\,. \tag{H.34}$$

Once again, we have a linear differential equation that allows us to superpose solutions. This turns out particularly convenient for BH initial data since it not only allows us to superpose multiple BHs but also different features of each BH. To see how this is achieved, we start with solutions X^i that carry angular momentum.

Proposition: The momentum constraint equation (H.34) for Bowen-York data is solved by

$$X^i = \epsilon^{ijk} \frac{x_j}{r^3} J_k \,, \tag{H.35}$$

where ϵ^{ijk} is the totally antisymmetric Levi-Civita symbol (which equals the Levi-Civita tensor since we have a flat conformal metric) and J_k is a constant vector.

Proof. Using $\partial_i r = x_i/r$, we obtain

$$\partial_m X^i = \epsilon^{ijk} J_k \left(\frac{\delta_{jm}}{r^3} - \frac{3}{r^5} x_j x_m \right) \tag{H.36}$$

$$\Rightarrow \quad \partial_m X^m = e^{mjk} J_k \left(\frac{\delta_{jm}}{r^3} - \frac{3}{r^5} x_j x_m \right) = 0 \tag{H.37}$$

$$\begin{aligned} \wedge \quad \partial_l \partial_m X^i &= \epsilon^{ijk} J_k \left[-\frac{3}{r^4} \frac{\delta_{jm} x_l}{r} - \frac{3}{r^5} \left(\delta_{jl} x_m + \delta_{ml} x_j \right) + \frac{15}{r^6} \frac{x_l x_j x_m}{r} \right] \\ &= \epsilon^{ijk} J_k \left[-\frac{3}{r^5} \left(\delta_{jm} x_l + \delta_{jl} x_m + \delta_{ml} x_j \right) + \frac{15}{r^7} x_j x_l x_m \right] \\ \Rightarrow \quad \partial^m \partial_m X^i &= \epsilon^{ijk} J_k \left[-\frac{3}{r^5} \left(x_j + x_j + 3x_j \right) + \frac{15}{r^7} r^2 x_j \right] = \epsilon^{ijk} J_k \left[-\frac{15 x_j}{r^5} + 15 \frac{x_j}{r^5} \right] = 0 \,. \end{aligned}$$

So both terms in the middle of Eq. (H.34) vanish individually. □

The extrinsic curvature is readily computed for this vector potential. We start with Eq. (H.33) where the last term vanishes by Eq. (H.37), so that

$$\begin{aligned} \bar{A}^{ij} &= \partial^j X^i + \partial^i X^j \overset{(H.36)}{=} \epsilon^{ink} J_k \left(\frac{\delta_n{}^j}{r^3} - \frac{3}{r^5} x_n x^j \right) + \epsilon^{jnk} J_k \left(\frac{\delta_n{}^i}{r^3} - \frac{3}{r^5} x_n x^i \right) \\ &= -\frac{3 x_n}{r^5} J_k \left(\epsilon^{ink} x^j + \epsilon^{jnk} x^i \right) \end{aligned} \tag{H.38}$$

$$\Rightarrow \quad K_{ij} = A_{ij} + \frac{1}{3} \gamma_{ij} K = \psi^{-2} \bar{A}_{ij} = -\frac{3 x_n}{r^5} J_k \psi^{-2} \left(\epsilon_i{}^{nk} x_j + \epsilon_j{}^{nk} x_i \right) \,. \tag{H.39}$$

For asymptotically flat spacetimes, the total angular momentum of the spacetime can now be computed from Eq. (8.83) of Ref. [24],

$$J_m^\infty = \frac{1}{8\pi} \lim_{r \to \infty} \oint_{S_r} (K_{ij} - K \gamma_{ij}) (\boldsymbol{\phi_m})^i \frac{x^j}{r} r^2 \sin\theta \mathrm{d}\theta \mathrm{d}\phi \,, \tag{H.40}$$

where S_r is the sphere of radius r and

$$\left.\begin{array}{lcl} \boldsymbol{\phi_x} = -z\partial_y + y\partial_z & \Leftrightarrow & (\boldsymbol{\phi_x})^i = (0,\ -z,\ y) \\ \boldsymbol{\phi_y} = -x\partial_z + z\partial_x & \Leftrightarrow & (\boldsymbol{\phi_y})^i = (z,\ 0,\ -x) \\ \boldsymbol{\phi_z} = -y\partial_x + x\partial_y & \Leftrightarrow & (\boldsymbol{\phi_z})^i = (-y,\ x,\ 0) \end{array}\right\} \Leftrightarrow \left\{\begin{array}{l} \qquad \boldsymbol{\phi_m} = \epsilon_{mj}{}^k x^j \boldsymbol{\partial}_k \\ \Rightarrow\ (\boldsymbol{\phi_m})^i = \boldsymbol{\phi_m}(\mathbf{d}x^i) = \epsilon_{mj}{}^k x^j \delta_k{}^i \\ \Rightarrow\ (\boldsymbol{\phi_m})^i = \epsilon_{mj}{}^i x^j \end{array}\right. . \tag{H.41}$$

Note that the integrand $(K_{ij} - K\gamma_{ij})(\boldsymbol{\phi_m})^i x^j / r$ is a scalar[14] and therefore can be evaluated in Cartesian coordinates even though we use spherical polar coordinates for the integration over the sphere. For the evaluation of this integrand, we need the product of two Levi-Civita tensors which in three dimensions for a Riemannian metric is given by

$$\epsilon_{ijk}\epsilon^{lmn} = \delta_i{}^l\delta_j{}^m\delta_k{}^n + \delta_i{}^m\delta_j{}^n\delta_k{}^l + \delta_i{}^n\delta_j{}^l\delta_k{}^m - \delta_i{}^l\delta_j{}^n\delta_k{}^m - \delta_i{}^n\delta_j{}^m\delta_k{}^l - \delta_i{}^m\delta_j{}^l\delta_k{}^n$$

$$\Rightarrow\ \epsilon_{ijk}\epsilon^{imn} = 3\delta_j{}^m\delta_k{}^n + \delta_j{}^n\delta_k{}^m + \delta_j{}^n\delta_k{}^m - 3\delta_j{}^n\delta_k{}^m - \delta_k{}^n\delta_j{}^m - \delta_j{}^m\delta_k{}^n \ = \ \delta_j{}^m\delta_k{}^n - \delta_j{}^n\delta_k{}^m \,.$$

For asymptotically flat spacetimes

$$\lim_{r\to\infty}\psi = 1 \qquad \Rightarrow \qquad \lim_{r\to\infty} K_{ij} = \bar{A}_{ij}\,, \tag{H.42}$$

and together with the condition $K = 0$, we can write the integrand in Eq.(H.40) as

$$\begin{aligned} \bar{A}_{ij}(\boldsymbol{\phi_m})^i x^j &= \bar{A}_{ij}\epsilon_{ml}{}^i x^l x^j \\ &= -\frac{3}{r^5} J_k \left[\epsilon_i{}^{nk} x_n x_j \epsilon_{ml}{}^i x^l x^j + \epsilon_j{}^{nk} x_n x_i \epsilon_{ml}{}^i x^l x^j\right] \\ &= -\frac{3}{r^5}\delta_{ms}\left[\epsilon_{ink}\epsilon^{isl} x^n x_j x_l x^j J^k + 0\right] \ = \ -\frac{3}{r^3}\left[(\delta_{nm}\delta_k{}^l - \delta_n{}^l\delta_{km}) x^n x_l J^k\right] \\ &= -\frac{3}{r^3}\left(x_m x_k J^k - x^l x_l J_m\right) \ = \ \frac{3}{r}\left(J_m - \frac{x_m x_k}{r^2} J^k\right) . \end{aligned} \tag{H.43}$$

Next, we use the freedom that we can always rotate our coordinate system such that J^k points in the z direction. With $J^k = (0,\ 0,\ J)$, we obtain

$$x^m x_k J^k = (xzJ,\ yzJ,\ z^2 J)\,, \qquad \text{and} \qquad x^l x_l J^m = (0,\ 0,\ r^2 J)\,. \tag{H.44}$$

With these expressions, Eq. (H.40) returns $J_x^\infty = J_y^\infty = 0$ because the integrand is $\sim z \sim \cos\theta$ which is odd across $\theta = \frac{\pi}{2}$. For the z component, on the other hand, we get

$$J_z^\infty = \lim_{r\to\infty}\frac{1}{8\pi}\oint_{S_r}\left(\frac{3}{r}J - \frac{3}{r^3}z^2 J\right) r\sin\theta \mathrm{d}\theta\mathrm{d}\phi = \lim_{r\to\infty}\frac{1}{8\pi}\oint_{S_r} 3J(1-\cos^2\theta)\sin\theta\mathrm{d}\theta\mathrm{d}\phi\,. \tag{H.45}$$

With

$$\int_0^\pi \sin\theta\mathrm{d}\theta = [-\cos\theta]_0^\pi = 2\,, \tag{H.46}$$

[14] The coordinate x^j is not a proper vector, but the outgoing unit normal vector on the sphere x^j/r is.

$$\int_0^\pi \sin\theta(1-\cos^2\theta)\mathrm{d}\theta = 2 - \int_0^\pi \cos^2\theta\,\sin\theta\mathrm{d}\theta = 2 + \left[\frac{1}{3}\cos^3\theta\right]_0^\pi = 2 - \frac{2}{3} = \frac{4}{3}\,,$$

we get $J_z^\infty = J$, so the vector parameter J_k in our vector potential (H.35) represents the angular momentum. So Eq. (H.35) gives us an extrinsic curvature contribution with angular momentum. We will now consider an alternative solution that gives us linear momentum.

Proposition: The momentum constraint equation (H.34) for Bowen-York data is also solved by

$$X^i = -\frac{1}{4r}\left(7P^i + \frac{x^i x_k}{r^2}P^k\right)\,, \tag{H.47}$$

where P^i is a constant vector.

Proof. We again consider Eq. (H.34) and compute

$$\begin{aligned}
\partial_m X^i &= \frac{7}{4r^2}P^i\frac{x_m}{r} + \partial_m\left[-\frac{1}{4}\frac{x^i x_k}{r^3}P^k\right] = \frac{7}{4r^2}P^i\frac{x_m}{r} + \frac{3x^i x_k x_m}{4r^5}P^k - \frac{1}{4}\frac{\delta^i{}_m x_k + x^i\delta_{km}}{r^3}P^k \\
&= \frac{7}{4}P^i\frac{x_m}{r^3} + \frac{3x^i x_k x_m}{4r^5}P^k - \frac{\delta^i{}_m x_k P^k + x^i P_m}{4r^3} \qquad \text{(H.48)}\\
\Rightarrow\ \partial_m X^m &= \frac{7}{4}P^m\frac{x_m}{r^3} + \frac{3x_k P^k}{4r^3} - \frac{3x_k P^k + x^m P_m}{4r^3} = \frac{3}{2}\frac{x_m P^m}{r^3} \qquad \text{(H.49)}\\
\wedge\ \partial_l\partial_m X^i &= \frac{7}{4}P^i\left[\frac{\delta_{ml}}{r^3} - 3\frac{x_m x_l}{r^5}\right] + \frac{3}{4}P^k\left[\frac{\delta^i{}_l x_k x_m}{r^5} + \frac{x^i\delta_{kl}x_m}{r^5} + \frac{x^i x_k\delta_{ml}}{r^5} - 5\frac{x^i x_k x_m x_l}{r^7}\right]\\
&\quad -\frac{1}{4}\left[\frac{\delta^i{}_m\delta_{kl}P^k}{r^3} - 3\frac{\delta^i{}_m x_k P^k x_l}{r^5} + \frac{\delta^i{}_l P_m}{r^3} - 3\frac{x^i P_m x_l}{r^5}\right]\\
\Rightarrow\ \partial^m\partial_m X^i &= \frac{7}{4}P^i\left[\frac{3}{r^3} - 3\frac{1}{r^3}\right] + \frac{3}{4}P^k\left[\frac{x_k x^i}{r^5} + \frac{x^i x_k}{r^5} + \frac{3x^i x_k}{r^5} - 5\frac{x^i x_k}{r^5}\right]\\
&\quad -\frac{1}{4}\left[\frac{P^i}{r^3} - 3\frac{x^i x_k P^k}{r^5} + \frac{P^i}{r^3} - 3\frac{x^i x_m P^m}{r^5}\right] = \frac{1}{2}\left[3\frac{x^i x_k P^k}{r^5} - \frac{P^i}{r^3}\right]\\
\wedge\ \partial^i\partial_m X^m &= \frac{3}{2}P^m\left[\frac{\delta^i{}_m}{r^3} - 3\frac{x_m x^i}{r^5}\right] = \frac{3}{2}\left[\frac{P^i}{r^3} - 3\frac{x^i x_m P^m}{r^5}\right]\\
\Rightarrow\ \partial^m\partial_m X^i + \frac{1}{3}\partial^i\partial_m X^m &= 0\,. \qquad \text{(H.50)}
\end{aligned}$$

□

The extrinsic curvature for this vector potential is given by

$$\begin{aligned}
\partial_j X_i &\overset{(H.48)}{=} \frac{7}{4}P_{(i}\frac{x_{j)}}{r^3} + \frac{3x_{(i}x_{j)}x_k}{4r^5}P^k - \frac{\delta_{ij}x_k P^k + x_{(i}P_{j)}}{4r^3} = \frac{3}{2}P_{(i}\frac{x_{j)}}{r^3} + \frac{3}{4}\frac{x_{(i}x_{j)}x_k P^k}{r^5} - \frac{\delta_{ij}x_k P^k}{4r^3} \\
\partial_m X^m &\overset{(H.49)}{=} \frac{3}{2}\frac{x_m P^m}{r^3} \\
\Rightarrow\ \bar{A}_{ij} &= \frac{3}{2}\frac{P_i x_j + x_i P_j}{r^3} + \frac{3}{2}\frac{x_i x_j x_k}{r^5}P^k - \frac{1}{2}\frac{\delta_{ij}x_k P^k}{r^3} - \delta_{ij}\frac{x_m P^m}{4r^3} \\
&= \frac{3}{2r^3}\left[P_i x_j + x_i P_j + \left(\frac{x_i x_j}{r^2} - \delta_{ij}\right) x_m P^m\right] \qquad \text{(H.51)}
\end{aligned}$$

The total linear momentum of the spacetime can be computed from Eq. (8.78) of Ref. [24],

$$P_i^{\mathrm{ADM}} = \frac{1}{8\pi}\lim_{r\to\infty}\oint_{S_r}(K_{ik} - K\gamma_{ik})\frac{x^k}{r}r^2\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi\,. \qquad \text{(H.52)}$$

Using again $K = 0$ and asymptotic flatness with $\psi \to 1$ at infinity, we have $K_{ik} - K\gamma_{ik} = \bar{A}_{ik}$ and can write the integrand of Eq. (H.52) as

$$\bar{A}_{ik}x^k = \frac{3}{2r^3}\left[r^2 P^i + x_i P_k x^k + (x^i - x^i)x_m P^m\right] = \frac{3}{2r^3}P^k(r^2\delta_{ik} + x_i x_k)\,. \qquad \text{(H.53)}$$

Let us again rotate our coordinate system such that P^k points in the z direction, $P^k = (0,\ 0,\ P)$, so that

$$\bar{A}_{ik}x^k = \frac{3P}{2r^3}\left(xz,\ yz,\ r^2 + z^2\right)\,.$$

As before, integrands $\sim z \sim \cos\theta$ in Eq. (H.52) result in vanishing integrals since $\cos\theta$ is odd across $\theta = \frac{\pi}{2}$, so that $P_x = P_y = 0$, whereas

$$P_z^{\mathrm{ADM}} = \frac{1}{8\pi}\lim_{r\to\infty}\oint_{S_r}\frac{3P}{2}(1 + \cos^2\theta)\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi\,.$$

With our above result (H.46), we find

$$\int_0^\pi \sin\theta(1 + \cos^2\theta)\mathrm{d}\theta = 2 + \frac{2}{3} = \frac{8}{3}\,,$$

and

$$P_z^{\mathrm{ADM}} = \frac{1}{8\pi}2\pi\frac{8}{3}\frac{3}{2}P = P\,, \qquad \text{(H.54)}$$

so that the parameter vector P^k denotes the linear momentum. Does it also contribute to the total angular momentum? To see why it does not, we use Eqs. (H.53) and (H.41) to compute

$$\bar{A}_{ij}(\boldsymbol{\phi_m})^i x^j = \frac{3}{2r^3}P^k(r^2\delta_{ik} + x_i x_k)\epsilon_{ml}{}^i x^l = \frac{3}{2r}\epsilon_{mlk}x^l P^k\,.$$

For $P^k = (0,\, 0,\, P)$, this gives us

$$\bar{A}_{ij}(\boldsymbol{\phi_m})^i x^j = \frac{3P}{2r}(y,\, -x,\, 0)\,,$$

which, inserted into Eq. (H.40), gives us

$$J_m^\infty = \frac{1}{8\pi} \lim_{r\to\infty} \oint_{S_r} \bar{A}_{ik}(\boldsymbol{\phi_m})^i x^k\, r \sin\theta \mathrm{d}\theta\, \mathrm{d}\phi = 0\,, \tag{H.55}$$

since $\int_0^{2\pi} \cos\phi \mathrm{d}\phi = \int_0^{2\pi} \sin\phi \mathrm{d}\phi = 0$.

Likewise, the extrinsic curvature contribution (H.38) to the angular momentum,

$$\bar{A}_{ij} = -\frac{3x_n}{r^5} J_k \left(\epsilon_i{}^{nk} x_j + \epsilon_j{}^{nk} x_i\right) \qquad \Rightarrow \qquad \bar{A}_{ij} x^j = -\frac{3x_n}{r^3} J_k \epsilon_i{}^{nk}\,, \tag{H.56}$$

has zero linear momentum. We see that by again rotating the coordinate system such that $J^k = (0,\, 0,\, J)$, so that

$$\bar{A}_{ij} x^j = -\frac{3}{r^3}(y,\, -x,\, 0)\,,$$

which, inserted into Eq. (H.52) gives us

$$P_i^{\mathrm{ADM}} = \frac{1}{8\pi} \lim_{r\to\infty} \oint_{S_r} \bar{A}_{ik} x^k r \sin\theta\, \mathrm{d}\theta \mathrm{d}\phi = 0\,,$$

since again $\int_0^{2\pi} \cos\phi \mathrm{d}\phi = \int_0^{2\pi} \sin\phi \mathrm{d}\phi = 0$.

Let us summarize our findings so far.

- For $\bar{\gamma}_{ij} = \delta_{ij}$, $K = 0$ and $Q^{ij} = 0$, the momentum constraint reduces to the linear differential equation (H.34) for the vector potential.
- This equation has the solutions (H.35) and (H.47) that contribute angular momentum J^k and linear momentum P^k, respectively.
- We can superpose these solutions in two ways, (i) to construct combinations of (H.35) and (H.47) that carry angular *and* linear momentum and (ii) to add such combinations centered at different points, say x^i_{A} and x^i_{B}. These solutions will ultimately give us initial data for multiple BHs with spin and boost[15] .

The Bowen-York solutions (H.35) and (H.47) give us analytic solutions to the momentum constraints, but we still have to compute the conformal factor ψ from the Hamiltonian constraint (H.26)

$$\bar{H} = 8\partial^m \partial_m \psi + \psi^{-7} \bar{A}_{mn} \bar{A}^{mn}\,.$$

[15] The extrinsic curvature $\bar{A}_{ij}$ derived in the original Bowen & York paper [48] contains some extra terms which merely ensure isometry under reflection across a sphere, but do not change the momenta. These terms were regarded as beneficial for solving the Hamiltonian constraint at the time, but turn out to be not necessary in more recent methods to solve the Hamiltonian constraint, so that we can safely ignore them.

Solving this highly non-linear PDE is no longer possible through analytic means, but we can still simplify the numerical process considerably by exploiting the fact that we already know the solution for the special case $\bar{A}_{mn} = 0$, the Brill-Lindquist conformal factor (H.32),

$$\psi_{\rm BL} = 1 + \sum_{i=1}^{n} \frac{M_{(i)}}{2|\boldsymbol{r} - \boldsymbol{r}_{(i)}|}\,,$$

where $M_{(i)}$ were free parameters determining the mass of the $i^{\rm th}$ BH. We now make the Ansatz

$$\psi = \psi_{\rm BL} + u\,, \tag{H.57}$$

where u is the function we need to solve for and $\psi_{\rm BL}$ satisfies the Laplace equation $\partial^m \partial_m \psi_{\rm BL} = 0$. On the domain $\mathbb{R} \setminus \{0\}$, we therefore obtain

$$\begin{aligned} & 8\partial^m \partial_m u + (\psi_{\rm BL} + u)^{-7} \bar{A}_{mn} \bar{A}^{mn} = 0 \\ \Rightarrow\quad & \partial^m \partial_m u + \frac{\bar{A}_{mn}\bar{A}^{mn}}{8\psi_{\rm BL}^7} \left(1 + \frac{u}{\psi_{\rm BL}}\right)^{-7} = 0\,. \end{aligned} \tag{H.58}$$

For asymptotic flatness, we impose the boundary condition $u = 1 + \mathcal{O}(r^-1)$ as $r \to \infty$. Brandt & Brügmann [49] have shown that there then exist unique solutions u to Eq. (H.58) that are regular on all $\mathbb{R}^3$. The regularity of the function u implies in particular that near the puncture locations $\boldsymbol{r}_{(i)}$, the Brill-Lindquist contribution $\psi_{\rm BL}$ dominates the conformal factor, so that the BH character of the solutions is preserved. Superposing the Bowen-York solutions for multiple BHs centered at $x^i_{\rm A}$, $x^i_{\rm B}$, ... the data represent a snapshot of a spacetime containing n BHs with spin and boost given by the parameters $\boldsymbol{J}_{(i)}$ and $\boldsymbol{P}_{(i)}$. These solutions are commonly known as puncture data and are the most common type of initial data used for BH binary simulation. Highly efficient elliptic solvers have been developed for the calculation of ψ from Eq. (H.58), most notably Ansorg's spectral solver [50] which has been ported to many codes in the form of the `TwoPunctures` module; see e.g. [51].

We conclude our discussion of initial data with some comments on the limitations of puncture data and ongoing approaches to circumvent these.

- The conformal transverse traceless decomposition leading to the constraint equations (H.26) and (H.27) is not the only way to apply a conformal rearrangement of the constraint equations. The most popular alternatives are the *physical transverse traceless split* and the *conformal thin sandwich* method; more details about these can be found in the reviews [42, 24].
- Puncture data typically contain some other "stuff" besides the n BHs located at the punctures. This feature arises from the conformal flatness approximation. In particular, it has been shown that the Kerr spacetime does not admit conformally flat spatial slices [52]. Bowen-York puncture data for a single spinning BH can therefore not represent an initial snapshot of a quiescent rotating BH. Instead, it contains some additional field contributions which in practice manifest themselves as a brief burst of unphysical gravitational radiation, colloquially referred to as *junk radiation*.

- Whereas the junk radiation is only a relatively minor inconvenience for BHs with mild to moderate spin and/or boost and can be removed by cutting off early "contaminated" parts of the GW signal, it grows rapidly as the dimensionless spin and/or boost velocity get close to 1. In particular, Bowen-York data are limited to BHs with dimensionless spins $J/M^2 \lesssim 0.93$ [53]. In simple terms, further increasing the parameter J^k in Eq. (H.35) adds more angular momentum to the junk radiation rather than the BH. A similar feature is observed for boosts close to the speed of light. These observations have motivated adjustments to the Bowen-York construction or the construction of alternative, non-conformally flat initial data [54, 55, 56].

H.2 Gauge conditions

We have seen in Sec. D that the Einstein equations make no predictions about the metric components $g_{0\alpha}$ or, in the language of the 3+1 formalism, about the lapse and shift; cf. Eq. (F.81). Rather, we are free to specify these variables freely in fixing the gauge or coordinate freedom of GR. We can classify the methods to do so into four main categories.

1. We prescribe lapse α and shift β^i as functions of the spacetime coordinates (t, x^i).
2. We prescribe α and β^i in terms of other evolution variables such as the spatial metric's volume element $\gamma = \chi^{-3}$ or the BSSNOK variable $\tilde{\Gamma}^i$.
3. We can impose elliptic differential equations. A popular example is the *maximum* slicing condition $K = 0$. By combining Eqs. (F.96), (F.98) and (F.99), we find after a straightforward calculation that

$$\partial_t K = \beta^m \partial_m K - \gamma^{ij} D_i D_j \alpha + \alpha \left[K_{mn} K^{mn} - \Lambda + 4\pi (S + \rho) \right] = 0 \,. \tag{H.59}$$

   Setting $K = 0$ in this equation gives us the elliptic differential equation

$$\triangle \alpha \coloneqq \gamma^{ij} D_i D_j \alpha = \alpha \left[K_{mn} K^{mn} - \Lambda + 4\pi (\rho + S) \right] \,. \tag{H.60}$$

4. We can evolve the gauge variables α and β^i according to hyperbolic or parabolic differential equations.

H.2.1 What can go wrong?

Before discussing some of the choices in more detail, it will be instructive to demonstrate with a concrete example the dangers and problems that can arise in choosing coordinates. For this purpose, we recall the Kruskal-Szekeres coordinates for the Schwarzschild spacetime; see e.g. Chapter D in Ref. [57] for more details. Starting with the standard Schwarzschild BH metric

$$\mathrm{d}s^2 = -\left(1 - \frac{2M}{r}\right) \mathrm{d}t^2 + \left(1 - \frac{2M}{r}\right)^{-1} \mathrm{d}r^2 + r^2 (\mathrm{d}\theta^2 + \sin^2\theta \mathrm{d}\phi^2) \,, \tag{H.61}$$

we perform successive coordinate transformations

$$\bar{t} = t + 2M \ln |r - 2M| \,, \qquad \tilde{t} = t - 2M \ln |r - 2M| \,,$$

$$v = \bar{t} + r\,, \qquad u = \tilde{t} - r\,,$$

$$\hat{v} = e^{\frac{v}{4M}}\,, \qquad \hat{u} = -e^{-\frac{u}{4M}}\,,$$

$$\hat{t} = \frac{1}{2}(\hat{v} + \hat{u})\,, \qquad \hat{r} = \frac{1}{2}(\hat{v} - \hat{u})\,. \tag{H.62}$$

In the resulting coordinates $(\hat{t}, \hat{r})$, the metric becomes

$$\mathrm{d}s^2 = \frac{16M^2}{r} e^{-\frac{r}{2M}} (-\mathrm{d}\hat{t}^2 + \mathrm{d}\hat{r}^2) + r^2(\mathrm{d}\theta^2 + \sin^2\theta\,\mathrm{d}\phi^2)\,, \tag{H.63}$$

and slices of constant Schwarzschild time $t = \text{const}$ or radius $r = \text{const}$ are given by the equations

$$\boxed{\frac{\hat{t}}{\hat{r}} = \tanh\frac{t}{4M}} \quad \text{for } r > 2M \qquad \text{and} \qquad \boxed{\frac{\hat{r}}{\hat{t}} = \tanh\frac{t}{4M}} \quad \text{for } r < 2M\,,$$

$$\text{or} \quad \boxed{\hat{t}^2 - \hat{r}^2 = -e^{\frac{r}{2M}}(r - 2M) =: C(r)}\,. \tag{H.64}$$

The resulting Kruskal-Szekeres diagram is illustrated in Fig. 14 together with several slices of constant Schwarzschild time and radius. We summarize the key insights of this solution as follows.

- The spacetime adds a mirror image of the Schwarzschild BH in the form of a white hole and a second asymptotically flat region on the left, resulting in four regions in total.
- Null geodesics follow lines of $\hat{t} \pm \hat{r} = \text{const}$, i.e. 45 degree slopes in this diagram. This implies causal disconnection of the two asymptotically flat regions on the left and right.
- Slices $r = \text{const} > 2M$ are timelike whereas slices $r = \text{const} < 2M$ are spatial, i.e. r becomes a timelike coordinate inside the horizon.
- The region $t = 0,\ r \geq 2M$ in Schwarzschild coordinates is mapped either to the semi-hypersurface $\hat{t} = 0,\ \hat{r} > 0$ or that with $\hat{t} = 0,\ \hat{r} < 0$, depending on which of the two asymptotically flat ends we choose. The region $t = 0,\ r < 2M$ is mapped to the vertical curve $\hat{r} = 0$ bounded by the singularities $r = 0$.
- One can show that the hypersurface $t = 0$ of the isotropic Schwarzschild spacetime (H.31) is instead mapped to the complete slice $\hat{t} = 0,\ \hat{r} \in \mathbb{R}$ of the Kruskal diagram.

Let us now assume that we start our numerical evolution with the initial slice $\hat{t} = 0$ or, equivalently, isotropic Schwarzschild data at $t = 0$.

Proposition: With geodesic slicing $\alpha = 1$ and $\beta^i = 0$, a numerical evolution starting on the hypersurface $\hat{t} = 0$ will encounter the BH singularity at $r = 0$ after πM time units, as illustrated in Fig. 15.

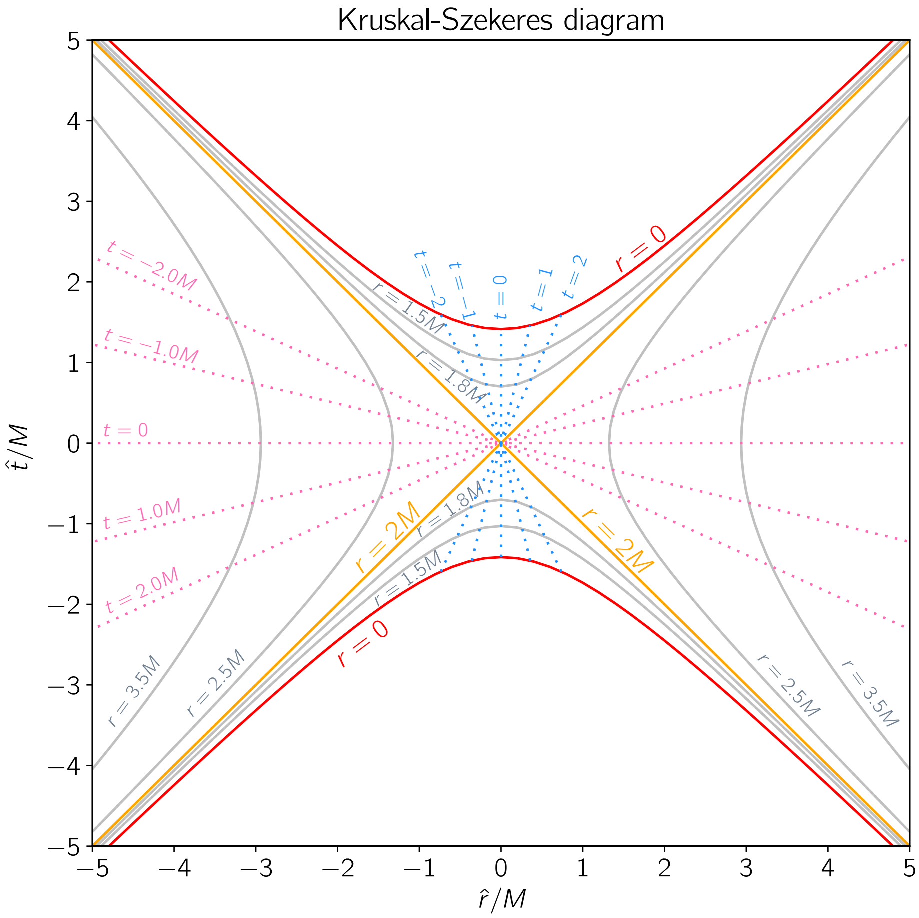


Figure 14: Kruskal-Szekeres diagram for the Schwarzschild BH with the singularity $r = 0$ marked in red, the horizon $r = 2M$ in orange and several slices of constant Schwarzschild time and radius in gray, magenta and sky blue. Each point represents a two-sphere with angles $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi)$.

Proof. The coordinate time of a numerical evolution is related to the proper time of observers moving with four-velocity n^μ by Eq. (F.84). Here we have $\alpha = 1$, so that $t_{\text{num}} = \tau$, assuming both are initialized as zero. We add here the subscript "num" to the coordinate time to distinguish it from the Schwarzschild coordinate t. Slices of constant coordinate time are therefore slices $\tau = \text{const}$.

Next, Eq. (F.51) tells us that the acceleration

$$a_\mu = n^\rho \nabla_\rho n_\mu = D_\mu \alpha = 0 \quad \text{for} \quad \alpha = 1\,, \tag{H.65}$$

so that the observers moving along n^μ are following geodesics, i.e. are freely falling. From the symmetry of the Kruskal-Szekeres diagram, we furthermore notice that at $\hat{t} = 0$, the derivative of the Schwarzschild radius along the normal direction n^μ vanishes, so our observers start with $\mathrm{d}r/\mathrm{d}\tau = 0$. We therefore need to compute the geodesics for observers starting at Schwarzschild

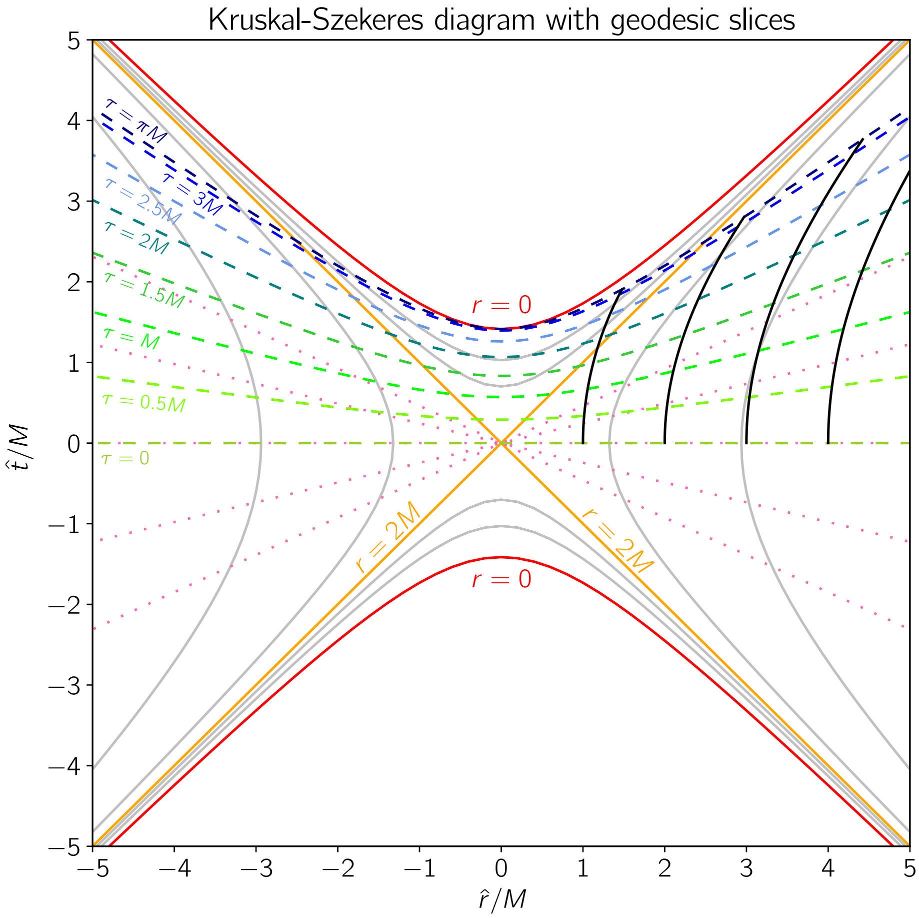


Figure 15: Kruskal-Szekeres diagram for the Schwarzschild BH with hypersurfaces of a numerical evolution starting at $\hat{t} = 0$ using geodesic slicing $\alpha = 1$ and vanishing shift vector $\beta^i = 0$. After πM units of evolution time, the hypersurfaces hits the singularity $r = 0$. The black solid curves display the trajectories of individual observers in the $(\hat{r}, \hat{t})$ plane spanned by the Kruskal-Szekeres coordinates.

time $t = 0$ from rest at initial radius $r \geq 2M$. Note that this corresponds to the semi-hypersurface $\hat{t} = 0$, $\hat{r} \geq 0$ in the Kruskal-Szekeres diagram; the evolution of observers starting at $\hat{r} < 0$ follows from symmetry across $\hat{r} = 0$.

Timelike geodesics with zero angular momentum in the Schwarzschild spacetime (H.61) are obtained from the equations (see for example chapter D4.2 in Ref. [57])

$$\left(1 - \frac{2M}{r}\right) \dot{t} = E \,, \qquad\qquad -E^2 + \dot{r}^2 = -1 + \frac{2M}{r} \,, \tag{H.66}$$

where $\dot{} := \mathrm{d}/\mathrm{d}\tau$ and E is a constant of motion determined by the initial conditions of the observer. Our observers start with $\dot{r} = 0$ at $r(0) = r_0$, so that

$$E = \sqrt{1 - \frac{2M}{r_0}} \in [0, 1) \quad \text{for} \quad r_0 \in [2M, \infty) \,,$$

$$\Rightarrow \quad \frac{\mathrm{d}r}{\mathrm{d}\tau} = \dot{r} = -\sqrt{\frac{2M}{r} - \frac{2M}{r_0}}\,,$$

where the negative root is used for infalling observers. Introducing the rescaled radius $x = r/r_0 \;\Leftrightarrow\; r = r_0 x$, obtain

$$r_0\dot{x} = -\sqrt{\frac{2M}{r_0}}\sqrt{\frac{1}{x} - 1}$$

$$\Rightarrow \quad \int\sqrt{\frac{x}{1-x}}\mathrm{d}x = -\sqrt{\frac{2M}{r_0^3}}\int \mathrm{d}\tau \tag{H.67}$$

The integral on the left is readily evaluated using substitutions,

$$u = \sqrt{x} \quad \Rightarrow \quad \mathrm{d}u = \frac{1}{2\sqrt{x}}\mathrm{d}x \quad \Rightarrow \quad 2u\mathrm{d}u = \mathrm{d}x$$

$$\Rightarrow \quad \int\frac{\sqrt{x}}{\sqrt{1-x}}\mathrm{d}x = \int\frac{u}{\sqrt{1-u^2}}2u\,\mathrm{d}u = 2\int\frac{u^2}{\sqrt{1-u^2}}\mathrm{d}u \qquad \Big| \quad u = \sin\xi \quad \Rightarrow \quad \mathrm{d}u = \cos\xi\,\mathrm{d}\xi$$

$$= 2\int\frac{\sin^2\xi}{\cos\xi}\cos\xi\,\mathrm{d}\xi = 2\int\sin^2\xi\,\mathrm{d}\xi = -\cos\xi\,\sin\xi + \xi = -u\sqrt{1-u^2} + \arcsin u$$

$$\Rightarrow \quad \boxed{\int\sqrt{\frac{x}{1-x}}\mathrm{d}x = -\sqrt{x(1-x)} + \arcsin\sqrt{x}}\,.$$

Equation (H.67) thus becomes

$$-\sqrt{\frac{2M}{r_0^3}}(\tau - \tau_0) = \left[-\sqrt{x(1-x)} + \arcsin\sqrt{x}\right]_1^{r/r_0} = \arcsin\sqrt{\frac{r}{r_0}} - \frac{\pi}{2} - \sqrt{\frac{r}{r_0}\left(1 - \frac{r}{r_0}\right)}$$

$$\Rightarrow \quad \tau = \underbrace{\tau_0}_{=0} + r_0\sqrt{\frac{r_0}{2M}}\left(\frac{\pi}{2} - \arcsin\sqrt{\frac{r}{r_0}}\right) + r_0\sqrt{\frac{r}{2M}}\sqrt{1 - \frac{r}{r_0}}\,, \tag{H.68}$$

and the singularity $r = 0$ is reached at $\tau = r_0\sqrt{r_0/(2M)}\pi/2$. The first observer to disintegrate in the singularity is the one starting at $r_0 = 2M$ after $\tau = \pi M$, presumably deriving little consolation from the shared destiny of her loyal followers whose demise is only marginally delayed thanks to their larger starting radius r_0. □

A numerical code exclusively operates with arrays of numbers and can therefore not represent the physical singularity at $r = 0$, where some or all evolution variables grow out of bounds. In practice, computer codes react to such situations by producing non-assigned numbers or[16]

[16]Some programming languages will print the partially capitalized version NaN we are using here while others print "nan" instead; of course it doesn't matter whether the doom of our simulation is spelled in lower or upper case.

"NaN"s. Without so-called NaN-checkers, computer codes will in fact happily continue crunching NaNs; to avoid wasting computational resources one should therefore check ones runs either using automated tools or by manually inspecting the log files.

Equation (H.68) gives us a neat analytic expression for the proper time of geodesic observers. In order to construct the slices in the Kruskal diagram, however, two further tasks need to be accomplished. First, we need to invert the relation $\tau(r)$ to obtain the radial position as a function of time, $r = r(\tau)$. This cannot be done in closed analytic form, but is straightforward to achieve numerically given the monotonic and smooth nature of $\tau(r)$. We use a Newton-Raphson[58] iteration which accomplishes this inversion with very high precision.

The second task involves more work; we need to compute one further variable along the observers' trajectories in order to determine their position in the $(\hat{t}, \hat{r})$ plane. The Schwarzschild time t is not suitable for this purpose, since it diverges at $r = 2M$, but we have multiple options for non-diverging coordinates such as $\bar{t}$ or $\hat{v}$. Unfortunately, the author has not found a variable that allows for analytic evaluation[17] as done in Eq. (H.68). We can, however, proceed with a relatively mild use of numerical methods; for this purpose, we inspect the evolution of the variable v in Eq. (H.62) which is given by

$$
\begin{aligned}
\mathrm{d}v &= \mathrm{d}\bar{t} + \mathrm{d}r = \mathrm{d}t + \frac{2M}{r-2M}\mathrm{d}r + \mathrm{d}r = \mathrm{d}t + \frac{r}{r-2M}\mathrm{d}r \\
\Rightarrow \quad \dot{v} &= \dot{t} + \frac{r}{r-2M}\dot{r} = E\frac{r}{r-2M} + \frac{r}{r-2M}\left(-\sqrt{\frac{2M}{r} - \frac{2M}{r_0}}\right) \\
&= \frac{r}{r-2M}\left[\sqrt{1-\frac{2M}{r_0}} - \sqrt{\frac{2M}{r} - \frac{2M}{r_0}}\right] . \qquad \text{(H.69)}
\end{aligned}
$$

Introducing the above rescaled radius $r = r_0 x$ as well as $a := 2M/r_0$, we can write this as

$$
\dot{v} = \frac{x}{x-a}\left[\sqrt{1-a} - \sqrt{\frac{a}{x} - a}\right] =: \frac{f}{g}\,, \qquad \text{(H.70)}
$$

with

$$
\begin{aligned}
f(x) &= \sqrt{1-a} - \sqrt{a}\sqrt{\tfrac{1}{x} - 1} \qquad \Rightarrow \qquad f'(x) = \frac{\sqrt{a}}{2x\sqrt{x}\sqrt{1-x}}\,, \\
g(x) &= \frac{x-a}{x} \qquad \Rightarrow \qquad g'(x) = \frac{a}{x^2}\,. \qquad \text{(H.71)}
\end{aligned}
$$

$\dot{v}$ has one singular point at $x = a$ which, however, is a removable singularity for $a > 1 \Leftrightarrow r_0 > 2M$ as we see with l'Hôpital's rule,

$$
\dot{v}\Big|_{x=a} = \frac{f}{g}\Big|_{x=a} = \frac{f'}{g'}\Big|_{x=a} = \frac{1}{2\sqrt{1-a}}\,. \qquad \text{(H.72)}
$$

[17] If someone knows such a variable, this would be welcome news.

For $r_0 > 2M$, we can therefore evaluate $v(\tau)$ by numerically integrating[18] Eq. (H.70) which gives us $v(\tau)$.

The case $r_0 = 2M$ is even simpler since by symmetry, this observer has to remain at $\hat{r} = 0$ which directly gives us her $\hat{t}(\tau)$ by inserting $r(\tau)$ into Eq. (H.64).

For all other observers, we have $r(\tau)$ and $v(\tau)$ along their journey which gives us their trajectory by computing through Eq. (H.62)

$$\hat{t} + \hat{r} = \hat{v} = e^{\frac{v}{4M}} \qquad \text{and} \qquad \hat{t}^2 - \hat{r}^2 = e^{-\frac{r}{2M}}(r - 2M)\,.$$

The slices thus obtained for an ensemble of observers is shown in Fig. 15 for several values of $\tau \in [0, \pi M]$. As we have already shown above, the observer starting at r_0 hits the singularity $r = 0$ at $\tau = \pi M$ unit. The solid black curves in the upper right quadrant of this figure show the trajectories of four specific observers; note that along their trajectories the Kruskal-Szekeres radius $\hat{r}$ increases but their Schwarzschild radius decreases (as expected for infalling observers).

We identify two key problems for the gauge choice of geodesic slicing and zero shift.

(A) The code reaches the singularity after πM time units and crashes by producing NaNs.

(B) A less evident problem is the gradual divergence of the individual observer's trajectories; see the four black solid lines in Fig. 15. This effect is known as *slice stretching* and implies that neighbouring grid points in a numerical implementation can separate to ever larger distance as time evolves. While not necessarily crashing a simulation, this can degrade the accuracy.

The first of these problems needs to be cured by better choices for the lapse function, the second is addressed by using non-zero shift vectors. Note in this context that the shift vector has no influence on the spacetime slicing. The surfaces $\tau = \text{const}$ in Fig. 15 look identical if we use a non-zero shift because the coordinate time of a numerical simulation is related to the proper time of observers moving with four velocity n^μ, irrespective of whether these observers have constant spatial coordinate position x^i in our numerical simulation; for $\beta^i = 0$ they do, but this is inconsequential for the proper time they measure as they advance from coordinate time t to $t + \mathrm{d}t$.

H.2.2 Singularity avoiding slicing

The key method that is used to address problem (A) in our above list is *singularity avoiding* slicing. The analysis of gauge condition is still an active area of research based on a combination of empirical findings and mathematical investigations. One of the most intensively studied scenario is the avoidance of singularities where the spatial volume element $\sqrt{\gamma} = \sqrt{\det \gamma_{ij}}$ vanishes. This is realized, for example, for the Schwarzschild metric in Kruskal-Szekeres coordinates (H.63) at r=0, but also occurs due to the focusing of the world lines of normal observers. We do not really care too much whether the vanishing of $\sqrt{\gamma}$ arises due to a physical singularity or merely a failure of the coordinates; either will break our simulations, so we seek for a way to avoid this happening. In doing so, we largely follow the work of Refs. [59, 60] which readers will find a good starting point for a more detailed discussion.

[18] The standard Trapezium rule works perfectly well for this simple problem.

The idea behind singularity avoiding slicing is to drive the lapse function α to zero in the vicinity of "dangerous regions" in the spacetime. From Eq. (F.84), we see that in that case, the proper time along the normal direction n^μ will slow down, essentially freezing the evolution near singular points while the simulation proceeds well and fine everywhere else in the spacetime. In terms of Fig. 15, a reduction of the lapse close to the singularity $r = 0$ means that slices of constant coordinate time t will freeze prior to reaching the singularity but continue evolving in the regions further away at larger $\hat{r}$. We therefore are looking for a way to prescribe the lapse function in a way that measures the local volume element $\sqrt{\gamma}$ and reduces α where γ becomes small.

Many of the slicing conditions employed in practical simulations are encompassed by the Bona-Massó family of hyperbolic slicing conditions introduced in the mid 90s [61].

Def. : In the Bona-Massó family of slicing conditions, the lapse function is evolved according to

$$\frac{\mathrm{d}\alpha}{\mathrm{d}t} := (\partial_t - \mathcal{L}_\beta)\alpha = (\partial_t - \beta^m\partial_m)\alpha = -\alpha^2 f(\alpha)K\,, \tag{H.73}$$

where $\mathcal{L}_\beta$ denotes the Lie derivative along the shift vector $\boldsymbol{\beta}$ and $f(\alpha)$ is a positive but otherwise free function.

It turns out convenient to derive an alternative representation of the Bona-Massó equation (H.73).

Lemma : In coordinates adapted to the 3+1 split, the components $\Gamma^0_{\mu\nu}$ of the spacetime Christoffel symbols can be written as

$$\Gamma^0_{00} = \frac{1}{\alpha}\left(\partial_0\alpha + \beta^m\partial_m\alpha\right) - \frac{1}{\alpha}\beta^m\beta^l K_{ml}\,, \tag{H.74}$$

$$\Gamma^0_{0i} = \frac{\partial_i\alpha}{\alpha} - \frac{1}{\alpha}\beta^m K_{im}\,, \tag{H.75}$$

$$\Gamma^0_{ij} = -\frac{1}{\alpha}K_{ij}\,. \tag{H.76}$$

Proof. The spacetime metric components in adapted coordinates are given by Eq. (F.81), so that

$$\begin{aligned}
\Gamma^0_{00} &= \frac{g^{0\rho}}{2}(\partial_0 g_{0\rho} + \partial_0 g_{\rho 0} - \partial_\rho g_{00}) = g^{0\rho}\left(\partial_0 g_{0\rho} - \frac{1}{2}\partial_\rho g_{00}\right) = \frac{g^{00}}{2}\partial_0 g_{00} + g^{0m}\left(\partial_0 g_{0m} - \frac{1}{2}\partial_m g_{00}\right) \\
&= -\alpha^{-2}\frac{1}{2}\partial_0(-\alpha^2 + \beta^m\beta_m) + \alpha^{-2}\beta^m\left[\partial_0\beta_m - \frac{1}{2}\partial_m(-\alpha^2 + \beta^n\beta_n)\right] \\
&= \frac{1}{2}\frac{2\alpha}{\alpha^2}\partial_0\alpha - \frac{1}{2\alpha^2}\left(\beta_m\partial_0\beta^m + \beta^m\partial_0\beta_m\right) + \frac{1}{\alpha^2}\beta^m\partial_0\beta_m - \frac{1}{2\alpha^2}\beta^m\left[-2\alpha\partial_m\alpha + \beta^n\partial_m\beta_n + \beta_n\partial_m\beta^n\right]
\end{aligned}$$

$$
\begin{aligned}
&= \frac{\partial_0\alpha}{\alpha} - \frac{1}{2\alpha^2}\beta_m\partial_0\beta^m - \frac{1}{2\alpha^2}\beta^m\partial_0\beta_m - \frac{1}{2\alpha^2}\beta^m\beta^n\partial_m\beta_n - \frac{1}{2\alpha^2}\beta^m\beta_n\partial_m\beta^n + \frac{1}{\alpha}\beta^m\partial_m\alpha + \frac{1}{\alpha^2}\beta^m\partial_0\beta_m \\
&= \frac{1}{\alpha}(\partial_0\alpha + \beta^m\partial_m\alpha) - \frac{1}{2\alpha^2}\left(\beta_m\partial_0\beta^m - \beta^m\partial_0\beta_m\right) - \frac{1}{2\alpha^2}\beta^m\left(\beta^n\partial_m\beta_n + \beta_n\partial_m\beta^n\right) \\
&= \frac{1}{\alpha}(\partial_0\alpha + \beta^m\partial_m\alpha) - \frac{1}{2\alpha^2}\Big(\beta_m\partial_0\beta^m - \gamma_{ml}\beta^m\partial_0\beta^l - \beta^m\beta^l\partial_0\gamma_{ml}\Big) \\
&\qquad - \frac{1}{2\alpha^2}\beta^m\Big(\beta^n\gamma_{nl}\partial_m\beta^l + \beta^n\beta^l\partial_m\gamma_{nl} + \beta_n\partial_m\beta^n\Big) \\
&= \frac{1}{\alpha}(\partial_0\alpha + \beta^m\partial_m\alpha) + \frac{1}{2\alpha^2}\beta^m\beta^l\partial_0\gamma_{ml} - \frac{1}{2\alpha^2}\beta^m\beta^n\beta^l\partial_m\gamma_{nl} - \frac{1}{\alpha^2}\beta^m\beta_l\partial_m\beta^l \\
&= \frac{1}{\alpha}(\partial_0\alpha + \beta^m\partial_m\alpha) + \frac{1}{2\alpha^2}\beta^n\beta^l\Big[2\gamma_{k(n}\partial_{l)}\beta^k - 2\alpha K_{nl}\Big] - \frac{1}{\alpha^2}\beta^m\beta_l\partial_m\beta^l \\
&= \frac{1}{\alpha}(\partial_0\alpha + \beta^m\partial_m\alpha) - \frac{1}{\alpha}\beta^m\beta^l K_{ml}\,. \qquad \text{(H.77)}
\end{aligned}
$$

For Γ^0_{0i}, we likewise find

$$
\begin{aligned}
\Gamma^0_{0i} &= \frac{1}{2}g^{0\rho}\left(\partial_0 g_{i\rho} + \partial_i g_{\rho 0} - \partial_\rho g_{0i}\right) \\
&= \frac{1}{2}g^{00}\left(\partial_0 g_{0i} + \partial_i g_{00} - \partial_0 g_{0i}\right) + \frac{1}{2}g^{0m}\left(\partial_0 g_{im} + \partial_i g_{m0} - \partial_m g_{0i}\right) \\
&= \frac{1}{2}g^{00}\partial_i g_{00} + \frac{1}{2}g^{0m}\left(\partial_0\gamma_{im} + \partial_i\beta_m - \partial_m\beta_i\right) \\
&= -\frac{1}{2\alpha^2}\partial_i(-\alpha^2 + \beta^m\beta_m) + \frac{1}{2\alpha^2}\beta^m\left(\partial_0\gamma_{im} + \partial_i\beta_m - \partial_m\beta_i\right) \\
&= \frac{\partial_i\alpha}{\alpha} - \frac{1}{2\alpha^2}\Big(\beta_m\partial_i\beta^m + \beta^m\partial_i\beta_m\Big) + \frac{1}{2\alpha^2}\beta^m\partial_0\gamma_{im} + \frac{1}{2\alpha^2}\beta^m\partial_i\beta_m - \frac{1}{2\alpha^2}\beta^m\partial_m\beta_i \\
&= \frac{\partial_i\alpha}{\alpha} - \frac{1}{2\alpha^2}\beta_m\partial_i\beta^m + \frac{1}{2\alpha^2}\beta^m\Big\{\beta^k\partial_k\gamma_{im} + \gamma_{ki}\partial_m\beta^k + \gamma_{km}\partial_i\beta^k - 2\alpha K_{im}\Big\} - \frac{1}{2\alpha^2}\beta^m\partial_m(\gamma_{il}\beta^l) \\
&= \frac{\partial_i\alpha}{\alpha} - \frac{1}{\alpha}\beta^m K_{im}\,. \qquad \text{(H.78)}
\end{aligned}
$$

Finally, we get

$$
\Gamma^0_{ij} = \frac{1}{2}g^{00}\left(\partial_i g_{j0} + \partial_j g_{0i} - \partial_0 g_{ij}\right) + \frac{1}{2}g^{0m}\left(\partial_i g_{jm} + \partial_j g_{mi} - \partial_m g_{ij}\right)
$$

$$
\begin{aligned}
&= -\frac{1}{2\alpha^2}\left(\partial_i\beta_j + \partial_j\beta_i - \partial_0\gamma_{ij}\right) + \frac{1}{2\alpha^2}\beta^m\left(\partial_i\gamma_{jm} + \partial_j\gamma_{mi} - \partial_m\gamma_{ij}\right) \\
&= \frac{1}{2\alpha^2}\left\{\gamma_{mi}\partial_j\beta^m + \gamma_{mj}\partial_i\beta^m - 2\alpha K_{ij}\right\} - \frac{1}{2\alpha^2}\partial_i(\gamma_{jm}\beta^m) - \frac{1}{2\alpha^2}\partial_j(\gamma_{im}\beta^m) \\
&\quad + \frac{1}{2\alpha^2}\beta^m\partial_i\gamma_{jm} + \frac{1}{2\alpha^2}\beta^m\partial_j\gamma_{im} \\
&= -\frac{1}{\alpha}K_{ij}\,. \qquad \text{(H.79)}
\end{aligned}
$$

□

Proposition: The Bona-Massó slicing condition (H.73) implies

$$
\left[g^{\mu\nu} + \left(1 - \frac{1}{f}\right)n^\mu n^\nu\right]\nabla_\mu\nabla_\nu t = 0\,, \qquad \text{(H.80)}
$$

Proof. First, we note that in adapted coordinates

$$
\nabla_\mu\nabla_\nu t = \partial_\mu\partial_\nu t - \Gamma^\rho_{\nu\mu}\partial_\rho t = \partial_\mu\delta^0{}_\nu - \Gamma^\rho_{\nu\mu}\delta^0{}_\rho = -\Gamma^0_{\mu\nu}\,. \qquad \text{(H.81)}
$$

Next, using $\gamma^{\alpha\beta} = g^{\alpha\beta} + n^\alpha n^\beta$, we obtain

$$
\begin{aligned}
-\left[g^{\mu\nu} + \left(1 - \frac{1}{f}\right)n^\mu n^\nu\right]\nabla_\mu\nabla_\nu t &= \gamma^{\mu\nu}\Gamma^0_{\mu\nu} - \frac{1}{f}n^\mu n^\nu\Gamma^0_{\mu\nu} \qquad \Big|\; n^\mu = \left(-\frac{1}{\alpha}, \frac{\beta^i}{\alpha}\right) \\
&= \gamma^{ij}\Gamma^0_{ij} - \frac{1}{f}\left(\frac{1}{\alpha^2}\Gamma^0_{00} - 2\frac{\beta^i}{\alpha^2}\Gamma^0_{0i} + \frac{\beta^i\beta^j}{\alpha^2}\Gamma^0_{ij}\right) \\
&= -\frac{\gamma^{ij}}{\alpha}K_{ij} - \frac{1}{f}\left[\frac{1}{\alpha^3}\partial_0\alpha + \frac{1}{\alpha^3}\beta^m\partial_m\alpha - \frac{1}{\alpha^3}\beta^m\beta^n K_{mn} - 2\frac{\beta^i}{\alpha^2}\left(\frac{\partial_i\alpha}{\alpha} - \frac{1}{\alpha}\beta^m K_{im}\right) - \frac{\beta^i\beta^j}{\alpha^2}\left(\frac{1}{\alpha}K_{ij}\right)\right] \\
&= -\frac{1}{\alpha}K - \frac{1}{f}\left[\frac{1}{\alpha^3}\left(\partial_0 - \beta^m\partial_m\right)\alpha\right] = -\frac{1}{f\alpha^3}\left[(\partial_0 - \beta^m\partial_m)\alpha + \alpha^2 f K\right] = 0\,, \qquad \text{(H.82)}
\end{aligned}
$$

where the terms in square brackets on the last line are exactly the Bona-Massó condition (H.73). □

The Bona-Massó family also turns out very convenient to analyze quantitatively how the lapse behaves in the neighbourhood of singularities. We illustrate this for so-called focusing singularities following Alcubierre [60].

Def. : A *focusing singularity* is a point where the volume element $\sqrt{\gamma}$ vanishes at a bounded rate as a function of the proper time measured by normal observers traveling with four-velocity n^μ.

The convenient nature of Bona-Massó slicing for analytic studies becomes clear if we consider the time evolution of the volume element γ. Recalling Eq. (G.51) for the conformal factor χ and its definition (G.36), we find

$$\begin{aligned}
(\partial_t - \beta^m\partial_m)\chi &= -\frac{2}{3}\chi\partial_m\beta^m + \frac{2}{3}\alpha\chi K \\
\Rightarrow\ (\partial_t - \beta^m\partial_m)\gamma^{1/2} &= (\partial_t - \beta^m\partial_m)\chi^{-3/2} = -\frac{3}{2}\chi^{-5/2}(\partial_t - \beta^m\partial_m)\chi = \chi^{-3/2}\partial_m\beta^m - \alpha\chi^{-3/2}K \\
\Rightarrow\ (\partial_t - \beta^m\partial_m)\gamma^{1/2} &= \gamma^{1/2}\partial_m\beta^m - \alpha\gamma^{1/2}K\,.
\end{aligned}$$

Recalling furthermore that the Lie derivative along a vector field $\boldsymbol{X}$ of a tensor density $\mathcal{T}^{\alpha\ldots}{}_{\beta\ldots}$ of weight w is

$$\mathcal{L}_{\boldsymbol{X}}\mathcal{T}^{\alpha\ldots}{}_{\beta\ldots} = X^\mu\partial_\mu\mathcal{T}^{\alpha\ldots}{}_{\beta\ldots} - (\partial_\mu X^\alpha)\mathcal{T}^{\mu\ldots}{}_{\beta\ldots} - \ldots + (\partial_\beta X^\mu)\mathcal{T}^{\alpha\ldots}{}_{\mu\ldots} + \ldots + w(\partial_\mu X^\mu)\mathcal{T}^{\alpha\ldots}{}_{\beta\ldots}\,,$$

we can write the evolution of the volume element as

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t}\gamma^{1/2} = (\partial_t - \mathcal{L}_{\boldsymbol{\beta}})\gamma^{1/2} = -\alpha\gamma^{1/2}K}\,. \tag{H.83}$$

Examples

(1) For $f(\alpha) = 1$, we obtain

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\alpha &= -\alpha^2 K \overset{(H.83)}{=} \frac{\alpha}{\sqrt{\gamma}}\frac{\mathrm{d}}{\mathrm{d}t}\sqrt{\gamma} \\
\Rightarrow\ \frac{\mathrm{d}}{\mathrm{d}t}\ln\alpha &= \frac{\mathrm{d}}{\mathrm{d}t}\ln\sqrt{\gamma} \\
\Rightarrow\ \alpha &= h(x^i)\sqrt{\gamma}\,,
\end{aligned} \tag{H.84}$$

where $h(x^i)$ is a function of integration that may depend on the spatial coordinates, but not on time. Setting $f = 1$ in Eq. (H.80), we see that this case corresponds to

$$\Box t = \nabla^\mu\nabla_\mu t = 0\,, \tag{H.85}$$

which is known as *harmonic slicing*. We will see below that it plays a special role in our classification of singularity avoidance.

(2) For $f(\alpha) = N = \text{const}$, we similarly obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\alpha = -\alpha^2 N K = \frac{\alpha N}{\sqrt{\gamma}}\frac{\mathrm{d}}{\mathrm{d}t}\sqrt{\gamma}$$

$$\Rightarrow \quad \ln\alpha = N\ln\sqrt{\gamma} + \tilde{h}(x^i)$$

$$\Rightarrow \quad \alpha = h(x^i)\sqrt{\gamma}^N\,. \tag{H.86}$$

(3) One of the most popular slicing conditions is obtained for $f = \frac{N}{\alpha}$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\alpha = -\alpha N K = \frac{N}{\sqrt{\gamma}}\frac{\mathrm{d}}{\mathrm{d}t}\sqrt{\gamma}$$

$$\Rightarrow \quad \alpha = h(x^i) + N\ln\sqrt{\gamma}\,. \tag{H.87}$$

For $h(x^i) = 1$ and $N = 2$, we obtain the special case

$$\frac{\mathrm{d}}{\mathrm{d}t}\alpha = \partial_t\alpha - \beta^m\partial_m\alpha = -2\alpha K \qquad \Rightarrow \qquad \alpha = 1 + \ln\gamma\,. \tag{H.88}$$

This class of gauge conditions is often referred to as "1+log" slicing, sometimes implying only the special case (H.88) and sometimes the more general Eq. (H.87). In particular, Eq. (H.88) is the slicing employed in most (if not all) moving puncture simulations, including the breakthroughs [8, 9].

(4) In the general case, we can still relate the volume element and the lapse through an integral equation,

$$\frac{\mathrm{d}}{\mathrm{d}t}\alpha = \frac{\alpha f}{\sqrt{\gamma}}\frac{\mathrm{d}}{\mathrm{d}t}\sqrt{\gamma}$$

$$\Rightarrow \quad \frac{1}{\alpha f}\frac{\mathrm{d}}{\mathrm{d}t}\alpha = \frac{1}{\sqrt{\gamma}}\frac{\mathrm{d}}{\mathrm{d}t}\sqrt{\gamma}$$

$$\Rightarrow \quad \boxed{\ln\sqrt{\gamma} + \tilde{h}(x^i) = \int\frac{1}{\alpha f(\alpha)}\frac{\mathrm{d}}{\mathrm{d}t}\alpha\mathrm{d}t = \int\frac{\mathrm{d}\alpha}{\alpha f(\alpha)}} \tag{H.89}$$

$$\Rightarrow \quad \boxed{\sqrt{\gamma} = h(x^i)\exp\left\{\int\frac{\mathrm{d}\alpha}{\alpha f(\alpha)}\right\}}\,. \tag{H.90}$$

The last two relations greatly help our analysis of the singularity avoidance. In particular, we already see that for finite $\alpha > 0$, the integral $\int\frac{\mathrm{d}\alpha}{\alpha f(\alpha)}$ is finite and γ cannot drop to zero. Read in reverse, this implies that Bona-Massó slicing will inevitably result in a "collapse of the lapse", i.e. $\alpha \to 0$, if the volume element shrinks to zero. We we will see below, this is a necessary, but not a sufficient condition for singularity avoidance.

Let us now assume that a focusing singularity is encountered at proper time τ_s as measured by a normal observer[19] Recalling that $\mathrm{d}\tau = \alpha \mathrm{d}t$, this corresponds to coordinate time

$$\Delta t = \int_0^{\tau_s} \frac{\mathrm{d}\tau}{\alpha} \tag{H.91}$$

We now have three possibilities.

(1) The volume element $\sqrt{\gamma}$ vanishes and α remains finite. As have just seen, this does not happen for Bona-Massó slicing.

(2) The lapse α vanishes as $\sqrt{\gamma}$ vanishes. In this case, the singularity may be reached at finite or infinite coordinate time, depending on the rate at which $\alpha \to 0$. If the singularity is reached at infinite coordinate time, we call this case *marginally singularity avoiding.*

(3) α vanishes before $\sqrt{\gamma}$ drops to zero. We call this case *strongly singularity avoiding.*

Let us now consider the concrete case

$$\begin{aligned} &\sqrt{\gamma} \sim (\tau_s - \tau)^m \quad \text{as} \quad \sqrt{\gamma} \text{ approaches } 0\,, \\ &f(\alpha) = A\alpha^n \qquad \text{as} \quad \alpha \text{ approaches } 0\,, \end{aligned} \tag{H.92}$$

where $A > 0$ for $f(\alpha) > 0$ and $m > 1$ to ensure $\sqrt{\gamma}$ vanishes at a bounded rate.

Proposition:

1. For $n < 0$, Bona-Massó slicing results in strong singularity avoidance.
2. For $n = 0$ and $mA \geq 1$, we have marginal singularity avoidance.
3. For $n > 0$ or $(n = 0$ and $mA < 1)$, the lapse collapses to zero at the singularity which, however, is reached at finite coordinate time, so that we have no singularity avoidance.

Proof. With Eq. (H.92), we obtain

$$\int \frac{\mathrm{d}\alpha}{\alpha f(\alpha)} = \frac{1}{A} \int \frac{\mathrm{d}\alpha}{\alpha^{n+1}} = \begin{cases} \ln\left(\alpha^{1/A}\right) & \text{for } n = 0 \\ -\frac{1}{An}\alpha^{-n} & \text{for } n \neq 0 \end{cases}.$$

Inserting the $n \neq 0$ case into Eq. (H.90) gives us

$$\sqrt{\gamma} = h(x^i) \exp\left\{\frac{-1}{nA}\alpha^{-n}\right\}.$$

For $n < 0$, this results in a finite γ as $\alpha \to 0$, so the lapse collapses before the singularity is reached. This proofs the first item in our proposition.

[19]Note that we always consider the proper time as measured by a normal observer. This is not necessarily the proper time measured along the integral curves of the timelike basis vector $\boldsymbol{\partial}_t$. The two integral curves coincide only for vanishing shift vector; cf. Fig. 13.

For $n \geq 0$, $\sqrt{\gamma}$ and α vanish simultaneously and we need to determine the coordinate time at which the singularity is reached. Recalling $\mathrm{d}\tau = \alpha \mathrm{d}t$, we get

$$\Delta t = \int_0^{\tau_s} \frac{\mathrm{d}\tau}{\alpha} = \int_{\alpha_0}^{0} \frac{\mathrm{d}\tau/\mathrm{d}\alpha}{\alpha} \mathrm{d}\alpha \,. \tag{H.93}$$

We have two possibilities:

(i) If $\frac{\mathrm{d}\tau}{\mathrm{d}\alpha}$ vanishes as α^p for some $p > 0$ or faster as $\alpha \to 0$, then the integral and, hence, Δt is finite, so that we have no singularity avoidance.

(ii) If $\frac{\mathrm{d}\tau}{\mathrm{d}\alpha}$ is finite or larger as $\alpha \to 0$, then the integral diverges, Δt is infinite and we have marginal singularity avoidance.

To calculate $\mathrm{d}\tau/\mathrm{d}\alpha$, we differentiate Eq. (H.89) with respect to proper time,

$$\frac{\mathrm{d} \ln \sqrt{\gamma}}{\mathrm{d}\tau} = \frac{1}{\alpha f} \frac{\mathrm{d}\alpha}{\mathrm{d}\tau} \,. \tag{H.94}$$

Inserting Eq. (H.92) leads to

$$\begin{aligned}
& \frac{\mathrm{d}}{\mathrm{d}\tau} \left[m \ln(\tau_s - \tau) \right] = \frac{1}{\alpha f} \frac{\mathrm{d}\alpha}{\mathrm{d}\tau} \\
\Rightarrow \quad & m \ln(\tau_s - \tau) = \int \frac{1}{\alpha f} \mathrm{d}\alpha \\
\Rightarrow \quad & \tau = \tau_s - \exp\left\{ \frac{1}{m} \int \frac{1}{\alpha f} \mathrm{d}\alpha \right\} \qquad \Big| \; f(\alpha) = A\alpha^n \\
& \quad = \tau_s - \exp\left\{ \frac{1}{mA} \int \frac{1}{\alpha^{n+1}} \mathrm{d}\alpha \right\} = \begin{cases} \tau_s - \left(\frac{\alpha}{\alpha_0}\right)^{\frac{1}{mA}} & \text{for } n = 0 \\ \tau_s - \exp\left[\frac{-1}{nmA}\left(\frac{1}{\alpha^n} - \frac{1}{\alpha_0^n}\right)\right] & \text{for } n > 0 \end{cases} .
\end{aligned}$$

- We first consider $n > 0$ which gives us

$$\frac{\mathrm{d}\tau}{\mathrm{d}\alpha} = -\exp\left[\frac{-1}{nmA}\left(\frac{1}{\alpha^n} - \frac{1}{\alpha_0^n}\right)\right] \frac{1}{mA} \frac{1}{\alpha^{n+1}} \,.$$

  As $\alpha \to 0$, this drops faster than α^p due to the exponential suppression, so Δt remains finite by Eq. (H.93) and we have no singularity avoidance.

- For $n = 0$, we obtain

$$\frac{\mathrm{d}\tau}{\mathrm{d}\alpha} = -\frac{1}{mA} \left(\frac{\alpha}{\alpha_0}\right)^{\frac{1}{mA} - 1} \xrightarrow{\alpha \to 0} \begin{cases} 0 & \text{if } mA < 1 \\ -1 & \text{if } mA = 1 \\ -\infty & \text{if } mA > 1 \end{cases} . \tag{H.95}$$

  The case $mA < 1$ gives us a power law falloff α^p, so that again Δt remains finite in Eq. (H.93) and we do not have singularity avoidance. The cases $mA \geq 1$, on the other hand, lead to a diverging Δt and are thus marginally singularity avoiding.

□

For $m=1$, i.e. a singularity $\sqrt{\gamma}\sim(\tau_s-\tau)$, the case $n=0$, $A=1$, i.e. the harmonic slicing condition $f(\alpha)=1$ from Example 1 on Page 148, marks the threshold between singularity avoidance and non-avoiding slicings.

H.2.3 Shift conditions

In our discussion of the normal observer's trajectories in the Kruskal diagram on Page 144, we have noticed the problem of slice stretching whereby the paths of neighbouring observers can deviate to increasingly large coordinate distance as time progresses. This effect is less catastrophic than the encounter of a singularity due to inappropriate slicing conditions, but can still have significant adverse effects on the performance of a code; as neighbouring grid points get far apart, discretization schemes may become inaccurate or even suffer from numerical instabilities. The methods for prescribing shift conditions to avoid this effect are on yet less solid mathematical ground than the derivation of singularity avoiding slicings, but they nonetheless work well in practice.

The exploration of "good" shift conditions dates back to the so-called *minimal-distortion shift condition* of Smarr & York [62]; see also Alcubierre *et al* [63] for a more recent discussion that we largely follow here. In simple terms, the idea is to introduce a measure for the divergent motion of neighbouring observers and prescribe the shift in a way that minimizes this quantity or, as is usually sufficient, to control and limit its growth.

Def. : The distortion tensor is

$$\Sigma_{ij}:=\frac{1}{2}\gamma^{1/3}\partial_t\tilde{\gamma}_{ij}=\frac{1}{2\chi}\partial_t\tilde{\gamma}_{ij}\,, \tag{H.96}$$

where γ, $\tilde{\gamma}_{ij}$ and χ are as defined in Eq. (G.36) for our BSSNOK variables.

The minimal distortion shift condition attempts to minimize the integral of $\Sigma_{mn}\Sigma^{mn}$ over the spatial hypersurface which leads to the elliptic differential equation (4.11) of Ref. [62],

$$D^j\Sigma_{ij}=0\qquad\Leftrightarrow\qquad D^j\left[D_i\beta_j+D_j\beta_i-\frac{2}{3}\gamma_{ij}D_k\beta^k\right]=D^j\left[2\alpha\left(K_{ij}-\frac{1}{3}\gamma_{ij}K\right)\right]\,. \tag{H.97}$$

We can intuitively interpret the distortion tensor as a measure for the change in the conformal metric weighted by the spatial volume element. By limiting or even minimizing the gradient of this quantity, we avoid neighbouring grid points drifting far apart. Unfortunately, the elliptic differential equation (H.97) is challenging and computationally costly to solve numerically, but with relatively minor adjustments, it leads to a highly convenient and successful evolution equation for the shift vector. To achieve this, we will establish a relation between the distortion tensor and the time derivative of the contracted conformal Christoffel symbols $\partial_t\tilde{\Gamma}^i$. We proceed in several steps.

Lemma : The distortion tensor can be written as

$$\Sigma^{ij} = \frac{\chi}{2}\left[-\beta^m\partial_m\tilde{\gamma}^{ij} + \tilde{\gamma}^{jl}\partial_l\beta^i + \tilde{\gamma}^{il}\partial_l\beta^j - \frac{2}{3}\tilde{\gamma}^{ij}\partial_m\beta^m - 2\alpha\tilde{A}^{ij}\right], \tag{H.98}$$

and it has zero trace,

$$\tilde{\gamma}_{mn}\Sigma^{mn} = 0\,. \tag{H.99}$$

Proof. Using Eq. (G.52) to replace $\partial_t\tilde{\gamma}_{ij}$ in the definition of the distortion tensor (H.96) gives us

$$\begin{aligned}
\Sigma^{ij} &= \gamma^{ik}\gamma^{jl}\Sigma_{kl} = \chi^2\tilde{\gamma}^{ik}\tilde{\gamma}^{jl}\frac{1}{2\chi}\partial_t\tilde{\gamma}_{kl} \\
&= \frac{\chi}{2}\tilde{\gamma}^{ik}\tilde{\gamma}^{jl}\left[\beta^r\partial_r\tilde{\gamma}_{kl} + \tilde{\gamma}_{mk}\partial_l\beta^m + \tilde{\gamma}_{ml}\partial_k\beta^m - \frac{2}{3}\tilde{\gamma}_{kl}\partial_m\beta^m - 2\alpha\tilde{A}_{kl}\right] \\
&= \frac{\chi}{2}\left[-\beta^m\partial_m\tilde{\gamma}^{ij} + \tilde{\gamma}^{jl}\partial_l\beta^i + \tilde{\gamma}^{ik}\partial_k\beta^j - \frac{2}{3}\tilde{\gamma}^{ij}\partial_m\beta^m - 2\alpha\tilde{A}^{ij}\right]
\end{aligned} \tag{H.100}$$

The vanishing trace is easiest to show using the unit determinant of the conformal metric whence $\partial_t\tilde{\gamma} = 0$ and therefore

$$\gamma^{ij}\Sigma_{ij} = \chi\tilde{\gamma}^{ij}\frac{1}{2\chi}\partial_t\tilde{\gamma}_{ij} = \frac{1}{2}\underbrace{\tilde{\gamma}^{ij}\partial_t\tilde{\gamma}_{ij}}_{=0} = 0\,. \tag{H.101}$$

□

Proposition: The distortion tensor is related to the contracted conformal Christoffel symbols by

$$2\partial_j(\chi^{-1}\Sigma^{ij}) = \frac{2}{\chi}\left(D_j\Sigma^{ij} - \tilde{\Gamma}^i_{jk}\Sigma^{jk} + \frac{3}{2}\frac{\partial_j\chi}{\chi}\Sigma^{ij}\right) = \partial_t\tilde{\Gamma}^i\,. \tag{H.102}$$

Proof. Using Eq. (G.38), we first compute

$$\begin{aligned}
D_j\Sigma^{ij} &= \partial_j\Sigma^{ij} + \Gamma^i_{mj}\Sigma^{mj} + \Gamma^j_{mj}\Sigma^{im} \\
&= \partial_j\Sigma^{ij} + \tilde{\Gamma}^i_{mj}\Sigma^{mj} + \underbrace{\tilde{\Gamma}^j_{mj}}_{=0}\Sigma^{im} - \frac{1}{2\chi}\left(\delta^i{}_j\partial_m\chi + \delta^i{}_m\partial_j\chi - \tilde{\gamma}_{mj}\tilde{\gamma}^{in}\partial_n\chi\right)\Sigma^{mj} \\
&\quad -\frac{1}{2\chi}\left(\delta^j{}_j\partial_m\chi + \delta^j{}_m\partial_j\chi - \tilde{\gamma}_{mj}\tilde{\gamma}^{jn}\partial_n\chi\right)\Sigma^{im}
\end{aligned}$$

$$= \partial_j \Sigma^{ij} + \tilde{\Gamma}^i_{mj}\Sigma^{mj} - \frac{1}{2\chi}\Big(5\partial_m\chi\Sigma^{mi} - \tilde{\gamma}^{in}\partial_n\chi\underbrace{\tilde{\gamma}_{mj}\Sigma^{mj}}_{=0}\Big)$$

$$= \partial_j \Sigma^{ij} + \tilde{\Gamma}^i_{mj}\Sigma^{mj} - \frac{5}{2\chi}\partial_m\chi\Sigma^{mi}\,. \tag{H.103}$$

Inserting this for $D_j\Sigma^{ij}$ in the middle term of Eq. (H.102), we get

$$\frac{2}{\chi}\left[D_j\Sigma^{ij} - \tilde{\Gamma}^i_{jk}\Sigma^{jk} + \frac{3}{2}\frac{\partial_j\chi}{\chi}\Sigma^{ij}\right] = \frac{2}{\chi}\left[\partial_j\Sigma^{ij} + \tilde{\Gamma}^i_{mj}\Sigma^{mj} - \frac{5}{2}\frac{\partial_m\chi}{\chi}\Sigma^{mi} - \tilde{\Gamma}^i_{jk}\Sigma^{jk} + \frac{3}{2}\frac{\partial_j\chi}{\chi}\Sigma^{ij}\right]$$

$$= \frac{2}{\chi}\left[\partial_j\Sigma^{ij} - \frac{\partial_m\chi}{\chi}\Sigma^{mi}\right] = 2\partial_j\left(\chi^{-1}\Sigma^{ij}\right)\,, \tag{H.104}$$

which proves the first equality in (H.102). For the second equality, we take the derivative of Eq. (H.98) and make some use of the identity $\tilde{\Gamma}^i = -\partial_m\tilde{\gamma}^{mi}$ from Eq. (G.41),

$$\begin{aligned}
2\partial_j(\chi^{-1}\Sigma^{ij}) &= -\partial_j(\beta^m\partial_m\tilde{\gamma}^{ij}) + \partial_j\tilde{\gamma}^{jl}\partial_l\beta^i + \tilde{\gamma}^{jl}\partial_j\partial_l\beta^i + \partial_j\tilde{\gamma}^{il}\partial_l\beta^j + \underline{\tilde{\gamma}^{il}\partial_j\partial_l\beta^j} \\
&\quad -\frac{2}{3}\partial_j\tilde{\gamma}^{ij}\partial_m\beta^m \underline{-\frac{2}{3}\tilde{\gamma}^{ij}\partial_j\partial_m\beta^m} - 2\partial_j\alpha\tilde{A}^{ij} - 2\alpha\partial_j\tilde{A}^{ij} \\
&= -\beta^m\partial_m(\partial_j\tilde{\gamma}^{ij}) \underline{-\partial_m\tilde{\gamma}^{ij}\partial_j\beta^m} - \tilde{\Gamma}^l\partial_l\beta^i + \tilde{\gamma}^{jl}\partial_j\partial_l\beta^i + \underline{\partial_j\tilde{\gamma}^{il}\partial_l\beta^j} + \frac{1}{3}\tilde{\gamma}^{im}\partial_m\partial_j\beta^j \\
&\quad +\frac{2}{3}\tilde{\Gamma}^i\partial_m\beta^m - 2\tilde{A}^{ij}\partial_j\alpha - 2\alpha\partial_j\tilde{A}^{ij} \\
&= \beta^m\partial_m\tilde{\Gamma}^i - \tilde{\Gamma}^l\partial_l\beta^i + \tilde{\gamma}^{jl}\partial_j\partial_l\beta^i + \frac{1}{3}\tilde{\gamma}^{im}\partial_m\partial_j\beta^j + \frac{2}{3}\tilde{\Gamma}^i\partial_m\beta^m - 2\tilde{A}^{ij}\partial_j\alpha - 2\alpha\partial_j\tilde{A}^{ij}\,.
\end{aligned}$$

For the final expression, we need the momentum constraint (G.50) in the form

$$\begin{aligned}
2\tilde{\gamma}^{im}M_m &= \frac{4}{3}\tilde{\gamma}^{im}\partial_m K - 2\tilde{D}_m\tilde{A}^{im} + 3\tilde{A}^{im}\frac{\partial_m\chi}{\chi} + 16\pi\tilde{\gamma}^{im}j_m = 0 \\
\Rightarrow\; -2\partial_m\tilde{A}^{im} &= 2\tilde{\Gamma}^i_{nm}\tilde{A}^{nm} + 2\underbrace{\tilde{\Gamma}^m_{nm}}_{=0}\tilde{A}^{in} - \frac{4}{3}\tilde{\gamma}^{im}\partial_m K - 3\tilde{A}^{im}\frac{\partial_m\chi}{\chi} - 16\pi\tilde{\gamma}^{im}j_m\,.
\end{aligned}$$

We use this result to replace the term $-2\alpha\partial_j\tilde{A}^{ij}$, so that

$$\begin{aligned}
2\partial_j(\chi^{-1}\Sigma^{ij}) &= \beta^m\partial_m\tilde{\Gamma}^i - \tilde{\Gamma}^l\partial_l\beta^i + \tilde{\gamma}^{jl}\partial_j\partial_l\beta^i + \frac{1}{3}\tilde{\gamma}^{im}\partial_m\partial_j\beta^j + \frac{2}{3}\tilde{\Gamma}^i\partial_m\beta^m - 2\tilde{A}^{ij}\partial_j\alpha \\
&\quad +\alpha\left(2\tilde{\Gamma}^i_{nm}\tilde{A}^{mn} - \frac{4}{3}\tilde{\gamma}^{im}\partial_m K - 3\tilde{A}^{im}\frac{\partial_m\chi}{\chi} - 16\pi\tilde{\gamma}^{im}j_m\right) \overset{(G.55)}{=} \partial_t\tilde{\Gamma}^i\,,
\end{aligned}$$

where the last equality arises from the evolution equation for $\tilde{\Gamma}^i$ dropping the auxiliary constraint term $\sigma\mathcal{G}^i$ which is zero in the continuum limit. □

Equation (H.102) motivates a modification of the minimal distortion shift condition by imposing $\partial_t\tilde{\Gamma}^i = 0$. This choice is known as the *Gamma freezing condition* and results in the elliptic equation obtained by setting the right-hand-side of Eq. (G.55) to zero which gives us a second-order elliptic PDE for β^i. It differs from the minimal distortion equation $D_j\Sigma^{ij} = 0$ only by terms containing first metric derivatives multiplied with the distortion tensor itself. In particular, the two equations do not differ in any terms involving second derivatives of β^i.

The Gamma freezing shift still involves solving a complicated PDE, but only on the initial hypersurface; afterwards, it can be maintained by simply not evolving the variable $\tilde{\Gamma}^i$. There is, however, an even more convenient way to achieve Gamma freezing shift without elliptic solving. The idea behind this approach is known as the *Gamma driver condition*. Driver type gauge conditions were introduced by Balakrishna *et al* [64] and inspired the Gamma driver established for BH evolutions by Alcubierre *et al* [63]. The idea is to source the evolution of the shift vector by $\partial_t\tilde{\Gamma}$ such that the shift ceases to change once Gamma freezing is achieved. In the parabolic version, this leads to

$$\partial_t\beta^i = F\partial_t\tilde{\Gamma}^i\,, \tag{H.105}$$

where F is a function of space and time. Empirically it has been observed that F needs to be positive to drive $\partial_t\tilde{\Gamma}^i$ towards the freezing condition. We can also construct a second-order shift condition,

$$\partial_t^2\beta^i = F\partial_t\tilde{\Gamma}^i - \tilde{\eta}\partial_t\beta^i\,, \tag{H.106}$$

where F and $\tilde{\eta}$ are functions of space and time that, again, need to be positive. Furthermore, in practical evolutions, the dissipation term $\tilde{\eta}\partial_t\beta^i$ is required to avoid oscillations of the shift. In particular the hyperbolic version has been employed with great success in the literature, typically in the form of a first order system with constant $F = 3/4$ and $M\eta = \mathcal{O}(1)$, where M is the ADM mass of the spacetime,

$$\partial_t\beta^i = \frac{3}{4}B^i\,, \qquad \partial_t B^i = \partial_t\tilde{\Gamma}^i - \eta B^i\,.$$

As a further adjustment, some evolutions replace the time derivative operator with the advection derivative $\partial_t - \beta^m\partial_m$. Together with the 1+log slicing condition (H.88), we can write this gauge choice as

$$\begin{aligned}
\partial_t\alpha &= \kappa\beta^m\partial_m\alpha - 2\alpha K\,,\\
\partial_t\beta^i &= \kappa\beta^m\partial_m\beta^i + \frac{3}{4}B^i\,,\\
\partial_t B^i &= \kappa\beta^m\partial_m B^i + (\partial_t - \kappa\beta^m\partial_m)\tilde{\Gamma}^i - \eta B^i\,.
\end{aligned} \tag{H.107}$$

Here κ is a parameter set to 0 or 1 to ex- or include the advection derivatives. These conditions are often referred to as *moving puncture gauge* since they are used with great success in the evolution of BH binaries starting with puncture data, including the moving puncture breakthroughs [8, 9].

That leaves us with just one question, how to initialize α and β^i? It turns out that the moving-puncture gauge is so robust that it works with a great variety of initial α and β^i. The most common choices are to start with vanishing shift and B^i as well as $\alpha = 1$ or $\alpha = \sqrt{\chi}$; other choices have, however, been used with comparable success. As a final comment, we note that the shift equations in (H.107) can be integrated analytically, resulting in

$$\partial_t \beta^i = \kappa \beta^m \partial_m \beta^i + \frac{3}{4}\tilde{\Gamma}^i - \eta \beta^i \,. \tag{H.108}$$

This condition is not necessarily equivalent to the second-order version in (H.107) due to integration constants, but also works very well in practice.

I Gravitational-wave diagnostics

In our final chapter, we discuss the extraction of gravitational waves and the corresponding radiated energy and momenta from numerical simulations. Here, we can be comparatively brief, since we have already done the hard work in Sec. E.

I.1 Gravitational-wave strain and the Newman-Penrose scalar

In Eqs. (E.102), (E.106) we have seen that in the limit $r \to \infty$, the GW strain can be expressed in terms of projections of the Riemann tensor according to

$$R_{\mu\nu\rho\sigma}\mathsf{k}^\mu \mathsf{m}^\nu \mathsf{k}^\rho \mathsf{m}^\sigma = -\frac{\mathrm{i}}{r}\partial_u^2 \bar{c} = -\frac{\mathrm{i}}{r}\partial_u^2\left(\frac{r}{2}h_+ - \mathrm{i}\frac{r}{2}h_\times\right) = -\frac{1}{2}(\mathrm{i}\partial_u^2 h_+ + \partial_u^2 h_\times)\,. \tag{I.1}$$

Here, $\mathbf{k}$ and $\mathbf{m}$ are part of a tetrad given by Eq. (E.98),

$$\mathbf{k} \simeq -\frac{1}{2}(\mathbf{e}_T - \mathbf{e}_R)\,, \qquad \boldsymbol{\ell} \simeq \mathbf{e}_T + \mathbf{e}_R\,, \qquad \mathbf{m} \simeq \frac{\mathbf{e}_\theta + \mathbf{e}_\phi}{2} + \mathrm{i}\frac{\mathbf{e}_\theta - \mathbf{e}_\phi}{2}\,. \tag{I.2}$$

In the more recent literature, it is common to work with a rescaled version of these tetrad vectors asymptotically related to the unit vectors $\mathbf{e}_T$, $\mathbf{e}_R$, $\mathbf{e}_\theta$ and $\mathbf{e}_\phi$ by

$$\tilde{\mathbf{k}} \simeq \frac{\mathbf{e}_T - \mathbf{e}_R}{\sqrt{2}}\,, \qquad \tilde{\boldsymbol{\ell}} \simeq \frac{\mathbf{e}_T + \mathbf{e}_R}{\sqrt{2}}\,, \qquad \widetilde{\mathbf{m}} \simeq \frac{\mathbf{e}_\theta + \mathrm{i}\mathbf{e}_\phi}{\sqrt{2}}\,. \tag{I.3}$$

This tetrad obeys the normalization

$$\boldsymbol{g}(\tilde{\mathbf{k}}, \tilde{\boldsymbol{\ell}}) = -1\,, \qquad \boldsymbol{g}(\widetilde{\mathbf{m}}, \overline{\widetilde{\mathbf{m}}}) = 1\,, \tag{I.4}$$

with all other inner products vanishing, and thus differs from Eq. (E.95) only by the minus sign in $\boldsymbol{g}(\tilde{\mathbf{k}}, \tilde{\boldsymbol{\ell}})$. Inverting Eq. (I.3) for the angular base vectors gives us

$$\begin{aligned}
\mathbf{e}_\theta &= \frac{\widetilde{\mathbf{m}} + \overline{\widetilde{\mathbf{m}}}}{\sqrt{2}}\,, \qquad \mathbf{e}_\phi = \frac{\widetilde{\mathbf{m}} - \overline{\widetilde{\mathbf{m}}}}{\sqrt{2}\mathrm{i}} = -\mathrm{i}\frac{\widetilde{\mathbf{m}} - \overline{\widetilde{\mathbf{m}}}}{\sqrt{2}} \\
\Rightarrow \quad \mathbf{m} &= \frac{1+\mathrm{i}}{2}\mathbf{e}_\theta + \frac{1-\mathrm{i}}{2}\mathbf{e}_\phi = \frac{1+\mathrm{i}}{2\sqrt{2}}(\widetilde{\mathbf{m}} + \overline{\widetilde{\mathbf{m}}}) + \frac{1-\mathrm{i}}{2\sqrt{2}}(-\mathrm{i})(\widetilde{\mathbf{m}} - \overline{\widetilde{\mathbf{m}}}) \\
&= \frac{1}{2\sqrt{2}}\left(\widetilde{\mathbf{m}} + \overline{\widetilde{\mathbf{m}}} + \mathrm{i}\widetilde{\mathbf{m}} + \mathrm{i}\overline{\widetilde{\mathbf{m}}} - \mathrm{i}\widetilde{\mathbf{m}} + \mathrm{i}\overline{\widetilde{\mathbf{m}}} - \widetilde{\mathbf{m}} + \overline{\widetilde{\mathbf{m}}}\right) = \frac{1}{2\sqrt{2}}\left(2\overline{\widetilde{\mathbf{m}}} + 2\mathrm{i}\overline{\widetilde{\mathbf{m}}}\right) \\
&= \frac{1+\mathrm{i}}{\sqrt{2}}\overline{\widetilde{\mathbf{m}}}\,.
\end{aligned} \tag{I.5}$$

Bearing also in mind that $\mathbf{k} = -\tilde{\mathbf{k}}/\sqrt{2}$, we can now rewrite Eq. (I.1) as

$$R_{\mu\nu\rho\sigma}\mathsf{k}^\mu \mathsf{m}^\nu \mathsf{k}^\rho \mathsf{m}^\sigma = R_{\mu\nu\rho\sigma}\frac{\tilde{\mathsf{k}}^\mu}{\sqrt{2}}\frac{1+\mathrm{i}}{\sqrt{2}}\overline{\widetilde{\mathsf{m}}}^\nu \frac{\tilde{\mathsf{k}}^\rho}{\sqrt{2}}\frac{1+\mathrm{i}}{\sqrt{2}}\overline{\widetilde{\mathsf{m}}}^\sigma = \frac{\mathrm{i}}{2}R_{\mu\nu\rho\sigma}\tilde{\mathsf{k}}^\mu\,\overline{\widetilde{\mathsf{m}}}^\nu\,\tilde{\mathsf{k}}^\rho\,\overline{\widetilde{\mathsf{m}}}^\sigma \tag{I.6}$$

In numerical relativity, it is more common to extract the GW signal in terms of the Newman-Penrose scalar Ψ_4 [65].

Def. : The Newman-Penrose scalar Ψ_4 is defined as[20]

$$\Psi_4 = C_{\mu\nu\rho\sigma}\tilde{\mathsf{k}}^{\mu}\,\overline{\tilde{\mathsf{m}}}^{\nu}\,\tilde{\mathsf{k}}^{\rho}\,\overline{\tilde{\mathsf{m}}}^{\sigma}\,, \tag{I.7}$$

where $C_{\mu\nu\rho\sigma}$ is the Weyl tensor related to the Riemann tensor in n spacetime dimensions by

$$C_{\alpha\beta\gamma\delta} = R_{\alpha\beta\gamma\delta} - \frac{2}{n-2}\left(g_{\alpha[\gamma}R_{\delta]\beta} - g_{\beta[\gamma}R_{\delta]\alpha}\right) + \frac{2}{(n-1)(n-2)}Rg_{\alpha[\gamma}g_{\delta]\beta}\,. \tag{I.8}$$

Proposition: In vacuum, Ψ_4 is related to the GW strain by

$$\Psi_4 = -\ddot{h}_+ + \mathrm{i}\ddot{h}_\times = \partial_T^2 H \qquad \text{with} \qquad H := -h_+ + \mathrm{i}h_\times\,. \tag{I.9}$$

Proof. In vacuum, the Riemann and Weyl tensors are equal, so that by Eqs. (I.1) and (I.6)

$$\Psi_4 \;=\; \frac{2}{\mathrm{i}}\left[-\frac{1}{2}(\mathrm{i}\partial_u^2 h_+ + \partial_u^2 h_\times)\right] \;=\; -\,\partial_u^2 h_+ + \mathrm{i}\partial_u^2 h_\times\,. \tag{I.10}$$

Furthermore, the derivatives with respect to retarded time $u = T - R$ and "normal" time are equal, $\partial_u = \partial_T$. □

I.2 Gravitational-wave energy and momentum

The energy and linear momentum carried by the GWs can be computed from the averaged stress energy tensor for the effective energy contained in high-frequency GWs first computed by Isaacson [66, 67] (see also [13] for more details). This tensor is constructed from second-order perturbation theory around the Minkowski spacetime and consists of the terms quadratic in the first order perturbations that appear on the right-hand side of the Einstein equations at second perturbative order. In terms of the trace reversed first-order perturbation, the Isaacson stress-energy tensor is given by

$$t_{\mu\nu} = \frac{1}{32\pi}\left\langle \partial_\mu \bar{h}_{\rho\sigma}\,\partial_\nu \bar{h}^{\rho\sigma} - \frac{1}{2}\partial_\mu \bar{h}\,\partial_\nu \bar{h} - 2\partial_\sigma \bar{h}^{\rho\sigma}\,\partial_{(\mu}\bar{h}_{\nu)\rho}\right\rangle\,. \tag{I.11}$$

Here $\langle\ .\ \rangle$ denotes the average over volumes that are large compared to the (cube of the) gravitational wave length. Crucially, $\langle t_{\mu\nu}\rangle$ can be shown to be gauge invariant, so that we can calculate it in the convenient transverse-traceless or "TT" gauge, where

$$t_{\mu\nu} = \frac{1}{32\pi}\langle \partial_\mu h_{ij}^{\mathrm{TT}}\,\partial_\nu h_{ij}^{\mathrm{TT}}\rangle\,, \tag{I.12}$$

[20] Some authors have an overall minus sign in the right-hand side of this definition of Ψ_4.

where we sum over i and j. We henceforth drop the superscript "TT" and implicitly assume that h_{ij} is given in the transverse traceless gauge.

The energy flux across a surface $x^k = \text{const}$ is given by

$$t^{0k} = \frac{1}{32\pi}\langle \partial^0 h_{ij}\, \partial^k h_{ij}\rangle = \frac{1}{32\pi}\langle -\partial_0 h_{ij}\, \partial_k h_{ij}\rangle\,. \tag{I.13}$$

The flux across a surface element $\mathrm{d}A$ with unit outgoing normal n_k is therefore given by

$$\frac{\mathrm{d}E}{\mathrm{d}t\,\mathrm{d}A} = t^{0k} n_k = \frac{1}{32\pi}\left\langle -\partial_0 h_{ij}\, \partial_k h_{ij}\, \frac{x_k}{R}\right\rangle = \frac{1}{32\pi}\left\langle -\partial_T h_{ij}\, \partial_R h_{ij}\right\rangle\,, \tag{I.14}$$

where we have used the outgoing unit normal for a surface element on a sphere of constant radius, $n_k = x_k/R$, and chain rule $(x_k/R)\partial_k = \partial_R$. In the limit $R\to\infty$, the perturbation h_{ij} is an outgoing plane wave and therefore a function of[21] $T-R$, so that $\partial_R h_{ij} = -\partial_T h_{ij}$ and

$$\frac{\mathrm{d}E}{\mathrm{d}t\,\mathrm{d}A} = \frac{1}{32\pi}\langle \partial_0 h_{ij}\, \partial_0 h_{ij}\rangle\,.$$

At each point on a sphere of constant radius R, we can rotate the Cartesian coordinates such that the z axis coincides with the radial direction, so that

$$h_{ij} = \begin{pmatrix} h_+ & h_\times & 0\\ h_\times & -h_+ & 0\\ 0 & 0 & 0\end{pmatrix} \qquad \Rightarrow \qquad \partial_0 h_{ij}\,\partial_0 h_{ij} = 2(\partial_0 h_+)^2 + 2(\partial_0 h_\times)^2$$

$$\Rightarrow \quad \frac{\mathrm{d}E}{\mathrm{d}t\,\mathrm{d}A} = \frac{1}{16\pi}\langle (\partial_0 h_+)^2 + (\partial_0 h_\times)^2\rangle\,. \tag{I.15}$$

Note that this is equivalent to Eq. (E.107) for the rate of change for the Bondi mass; of course, it is reassuring to obtain this agreement with the fully non-linear characteristic calculation. With $H = -h_+ + \mathrm{i}h_\times$ we obtain

$$|\partial_T H|^2 = \partial_T H\, \partial_T \bar{H} = (-\partial_T h_+ + \mathrm{i}\partial_T h_\times)(-\partial_T h_+ - \mathrm{i}\partial_T h_\times) = (\partial_T h_+)^2 + (\partial_T h_\times)^2$$

$$\overset{(I.9)}{=} \left|\int_{-\infty}^{T} \Psi_4 \mathrm{d}\tilde{t}\right|^2\,, \tag{I.16}$$

so that Eq. (I.15) gives us the total energy flux

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \lim_{R\to\infty}\frac{R^2}{16\pi}\oint |\partial_T H|^2 \mathrm{d}\Omega = \lim_{R\to\infty}\frac{R^2}{16\pi}\oint \left|\int_{-\infty}^{T}\Psi_4 \mathrm{d}\tilde{t}\right|^2 \mathrm{d}\Omega\,. \tag{I.17}$$

[21] There is a subtle issue here. Despite being a function of $T-R$, the perturbations will in general vary with the angular direction – otherwise, all GWs would be spherically symmetric which they cannot be due to Birkhoff's theorem. Derivatives transverse to the direction of propagation, however, are suppressed by the conversion from angular to Cartesian derivatives, as for example in $\partial_x = r_{,x}\partial_r + \theta_{,x}\partial_\theta + \phi_{,x}\partial_\phi$. Here, $\theta_{,x} := \partial\theta/\partial x = zx/(\rho R^2)$, $\phi_{,x} = -y/\rho^2$ with $\rho = \sqrt{x^2+y^2}$, so these derivatives decay $\propto 1/R$ and even for finite angular derivatives, derivatives of the wave in Cartesian coordinates vanish at $R\to\infty$ except in the direction of the wave propagation. It is for this reason that we can ignore angular derivatives and write $h_{ij} = h_{ij}(T-R)$.

For the linear momentum we use the relation

$$\frac{\partial}{\partial x^l}h_{ij} = \frac{\partial R}{\partial x^l}\partial_R h_{ij} + \frac{\partial \theta}{\partial x^l}\partial_\theta h_{ij} + \frac{\partial \phi}{\partial x^l}\partial_\phi h_{ij} \quad \overset{R\to\infty}{\longrightarrow} \quad \frac{\partial R}{\partial x^l}\partial_R h_{ij}\,,$$

which allows us to write

$$\frac{\mathrm{d}P^l}{\mathrm{d}t\,\mathrm{d}A} = t^{lk}n_k = \frac{1}{32\pi}\left\langle \partial_l h_{ij}\,\partial_k h_{ij}\frac{x^k}{r}\right\rangle = \frac{1}{32\pi}\left\langle \frac{x_l}{R}\partial_R h_{ij}\,\partial_R h_{ij}\right\rangle = \frac{1}{32\pi}n_l\langle \partial_T h_{ij}\,\partial_T h_{ij}\rangle\,. \tag{I.18}$$

Here, the components of the unit normal can be written as

$$n_l = \frac{x_l}{R} = (\sin\theta\cos\phi,\ \ \sin\theta\sin\phi,\ \ \cos\theta)\ . \tag{I.19}$$

Using Eq. (I.16), the total momentum flux becomes

$$\frac{\mathrm{d}P_l}{\mathrm{d}t} = \lim_{R\to\infty}\frac{R^2}{16\pi}\oint n_l|\partial_t H|^2\mathrm{d}\Omega = \lim_{R\to\infty}\frac{R^2}{16\pi}\oint n_l\left|\int_{-\infty}^{T}\Psi_4\mathrm{d}\tilde{t}\right|^2\mathrm{d}\Omega\,. \tag{I.20}$$

This proofs the following result.

Proposition: The energy and linear momentum carried by gravitational radiation is

$$\frac{\mathrm{d}E}{\mathrm{d}t}\lim_{R\to\infty}\frac{R^2}{16\pi}\oint|\partial_T H|^2\mathrm{d}\Omega = \lim_{R\to\infty}\frac{R^2}{16\pi}\oint\left|\int_{-\infty}^{T}\Psi_4\mathrm{d}\tilde{t}\right|^2\mathrm{d}\Omega \tag{I.21}$$

$$\frac{\mathrm{d}P_l}{\mathrm{d}t} = \lim_{R\to\infty}\frac{R^2}{16\pi}\oint n_l|\partial_t H|^2\mathrm{d}\Omega = \lim_{R\to\infty}\frac{R^2}{16\pi}\oint n_l\left|\int_{-\infty}^{T}\Psi_4\mathrm{d}\tilde{t}\right|^2\mathrm{d}\Omega\,,$$

$$\text{with}\quad n_l = (\sin\theta\cos\phi,\ \ \sin\theta\sin\phi,\ \ \cos\theta)\,. \tag{I.22}$$

Computing the angular momentum carried by the gravitational radiation is more involved since the averaging used for the derivation of the Isaacson stress energy tensor does not take into account contributions $\propto r^{-3}$ which are essential for the angular momentum. We only quote here the final result; see Ref. [68] for more details.

Proposition: The angular momentum carried by gravitational radiation is given by

$$\begin{aligned}\frac{\mathrm{d}J_i}{\mathrm{d}t} &= -\lim_{R\to\infty}\frac{R^2}{16\pi}\mathsf{Re}\left\{\oint \hat{J}_i H\,\partial_T\bar{H}\,\mathrm{d}\Omega\right\}\\ &= -\lim_{R\to\infty}\frac{R^2}{16\pi}\mathsf{Re}\left\{\oint \hat{J}_i\left(\int_{-\infty}^{T}\int_{-\infty}^{\hat{t}}\Psi_4\mathrm{d}\tilde{t}\,\mathrm{d}\hat{t}\right)\times\left(\int_{-\infty}^{T}\bar{\Psi}_4\mathrm{d}\tilde{t}\right)\right\}\,,\end{aligned}$$

$$\text{with}\quad \hat{J}_x = -\sin\phi\partial_\theta - \cos\phi\left(\cot\theta\partial_\phi - \frac{2\mathrm{i}}{\sin\theta}\right)\,,$$

$$\hat{J}_y = \cos\phi\partial_\theta - \sin\phi\left(\cot\theta\partial_\phi - \frac{2\mathrm{i}}{\sin\theta}\right)\qquad\text{and}\qquad \hat{J}_z = \partial_\phi\,. \tag{I.23}$$

I.3 The multipolar decomposition of Ψ_4

Gravitational wave signals are most commonly plotted as functions of one variable, typically time, sometimes frequency. These plots result from a multipolar decomposition of the signal which we summarize here for the Newman-Penrose scalar Ψ_4, but which works in complete analogy for the strain function H.

Given a GW signal $\Psi_4(T, R_{\rm ex}, \theta, \phi)$ extracted on a sphere of constant extraction radius $R_{\rm ex}$, we obtain the individual multipoles of indices $l = 2, 3, \ldots, m = -l, -l+1, \ldots, l$ by projecting Ψ_4 onto spherical harmonics Y^{-2}_{lm} of spin-weight -2,

$$\psi_{lm} := \langle Y^{-2}_{lm}, \Psi_4 \rangle := \int_0^{2\pi} \int_0^{\pi} \Psi_4 \bar{Y}^{-2}_{lm} \sin\theta \, \mathrm{d}\theta \, \mathrm{d}\phi \, .$$

$$\Rightarrow \quad \Psi_4(t, \theta, \phi) = \sum_{l=2}^{\infty} \sum_{m=-l}^{l} \psi_{lm}(t) Y^{-2}_{lm}(\theta, \phi) \, . \tag{I.24}$$

Ideally, the extraction and decomposition should be performed at $R_{\rm ex} \to \infty$, but in practice, it is commonly done at several large finite radii. The results at different radii can be extrapolated to infinity, either in an attempt to improve the result or to calibrate the uncertainties incurred when using finite $R_{\rm ex}$.

The spin-weighted spherical harmonics Y^{s}_{lm} for arbitrary weight s are defined in terms of the Wigner d functions (see e.g. Ref. [69]),

$$Y^s_{lm} = (-1)^s \sqrt{\frac{2l+1}{4\pi}} \, d^l_{m(-s)}(\theta) e^{\mathrm{i}m\phi} \, ,$$

$$\text{where} \quad d^l_{ms}(\theta) = \sum_{\kappa=C_1}^{C_2} \frac{(-1)^\kappa [(l+m)!(l-m)!(l+s)!(l-s)!}{(l+m-\kappa)!(l-s-\kappa)!\kappa!(\kappa+s-m)!} \left(\frac{\cos\theta}{2}\right)^{2l+m-s-2\kappa} \left(\frac{\sin\theta}{2}\right)^{2\kappa+s-m} \, ,$$

$$\text{with} \quad C_1 = \max(0, \, m-s) \, , \qquad C_2 = \min(l+m, \, l-s) \, . \tag{I.25}$$

For $l = 2$, for example, this results in

$$Y^{-2}_{22}(\theta, \phi) = \sqrt{\frac{5}{64\pi}} (1+\cos\theta)^2 e^{2\mathrm{i}\phi} \, ,$$

$$Y^{-2}_{21}(\theta, \phi) = \sqrt{\frac{5}{16\pi}} \sin\theta (1+\cos\theta) e^{\mathrm{i}\phi} \, ,$$

$$Y^{-2}_{20}(\theta, \phi) = \sqrt{\frac{15}{32\pi}} \sin^2\theta \, ,$$

$$Y^{-2}_{2-1}(\theta, \phi) = \sqrt{\frac{5}{16\pi}} \sin\theta (1-\cos\theta) e^{-\mathrm{i}\phi} \, ,$$

$$Y^{-2}_{2-2}(\theta,\phi) \;=\; \sqrt{\frac{5}{64\pi}}\,(1-\cos\theta)^2 e^{-2i\phi}\,. \tag{I.26}$$

The spherical harmonics form a complete orthonormal basis, so that

$$\langle Y^{-2}_{lm}, \bar{Y}^{-2}_{l'm'}\rangle = \langle \bar{Y}^{-2}_{lm}, Y^{-2}_{l'm'}\rangle = \delta_{ll'}\delta_{mm'}\,. \tag{I.27}$$

This allows us to determine the GW energy contained in individual modes by inserting the multipolar decomposition (I.24) into Eq. (I.21) for the radiated energy,

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \sum_{l,m}\dot{E}_{lm} \qquad \text{with} \qquad \dot{E}_{lm} = \lim_{R\to\infty}\frac{R^2}{16\pi}\left|\int_{-\infty}^{T}\psi_{lm}\mathrm{d}\tilde{t}\right|^2\,. \tag{I.28}$$

A similar analysis for the linear momentum is significantly more complicated and involves overlap integrals of different multipoles, so that a linear momentum contribution can only be assigned to a set of ≥ 2 modes rather than individual ones. Details of this calculation can be found in Sec. 3 of Ref. [70].

I.4 An example of a GW signal

Many of the topics of these notes have been actively employed in the calculation of a GW signal from the numerical simulation of a black-hole binary with mass ratio $q = 1:4$ inspiraling for about 11 orbits before merging into a single BH. This simulation has used the BSSNOK formulation of Sec. G.3 together with the moving puncture gauge conditions (H.107); for more details see Ref. [71]. In Fig. 16 we show the real parts of the leading multipoles of the GW strain extracted at two different extraction radii together with the extrapolation to $R_{\rm ex}\to\infty$. The imaginary parts look identical up to a 90° phase shift. Here the multipoles are defined in complete analogy to Eq. (I.24) by

$$H_{lm} = \langle Y^{-2}_{lm}, H\rangle = \int_0^{2\pi}\int_0^{\pi} H\bar{Y}^{-2}_{lm}\,\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi\,. \tag{I.29}$$

Note that the second and third strongest multipoles H_{32} and H_{42} are amplified by factors of 40 and 400, respectively, in the figure, demonstrating that the signal is dominated by the $(2,2)$ and $(2,-2)$ quadrupoles; H_{2-2}, which equals $\bar{H}_{22}$ for this binary, is not shown in the figure to avoid overcrowding.

Calculations of this type played a key role in the first detection of a gravitational-wave signal by LIGO in 2015 [11]. This discovery was awarded the 2017 Nobel Prize and has inaugurated the new research field of GW astronomy. The methodology summarized in these lecture notes remains an essential technology to make theoretical predictions about astrophysical sources of GWs that provide us with the GW analog of a finger print data base that we can compare with actual observations to try and identify the signals' origins in the Universe.

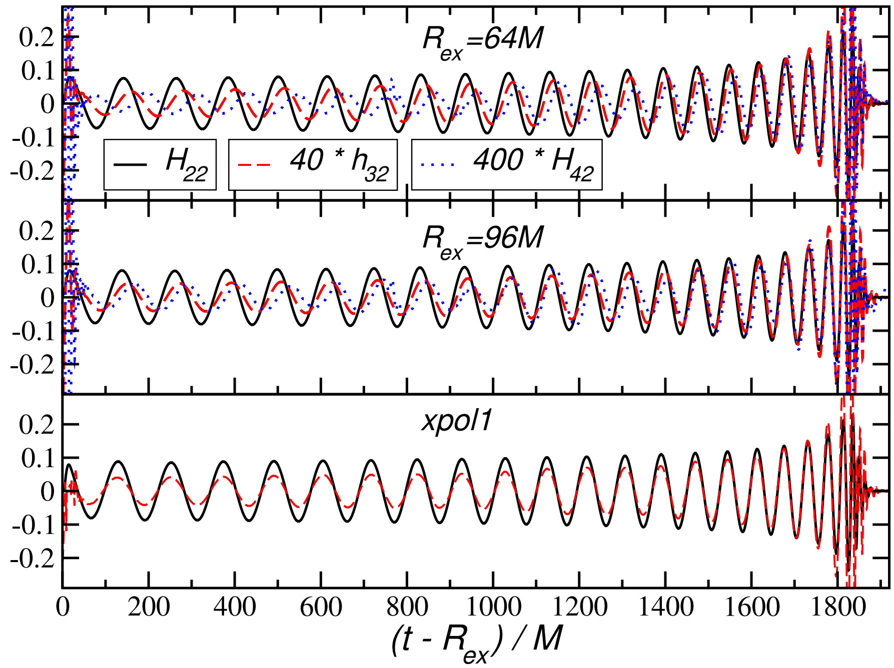


Figure 16: The real parts of some GW multipoles $(R_{\rm ex}/M)\,H_{lm}$ are plotted for an 11 orbit inspiral of a non-spinning BH binary with mass ratio 1 : 4 is plotted as a function of retarded time. The different panels show the signals extracted at $R_{\rm ex} = 64\,M$ and $96\,M$ as well as extrapolated to infinite extraction radius. Note that the subdominant H_{32} and H_{42} are amplified by factors of 40 and 400, respectively; the signal is dominated by the quadrupole modes H_{22} and H_{2-2} (not shown here).

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