Abstract.

This paper gives a detailed pedagogic presentation of the central concepts underlying a new algorithm for the numerical solution of Einstein’s equations for gravitation. This approach incorporates the best features of the two leading approaches to computational gravitation, carving up spacetime via Cauchy hypersurfaces within a central worldtube, and using characteristic hypersurfaces in its exterior to connect this region with null infinity and study gravitational radiation. It has worked well in simplified test problems, and is currently being used to build computer codes to simulate black hole collisions in 3-D.

1. Preamble

Throughout his career in theoretical gravitational physics, Vishnu has been interested in questions of black holes and gravitational radiation. The subject of his useful early study of radiation from binary systems [1] is now at
the forefront of research as the principal target for the first exciting experimental measurements of the LIGO project. His fundamental studies of the properties of black hole excitations and radiation [2] used the formidable technology of the mid 1960's, i.e. Regge-Wheeler perturbation theory, to analytically extract the crucial physical result that black holes were stable. In his continuing studies of the interaction of black holes with gravitational radiation [3], he first demonstrated the phenomenon that was later to be called normal mode excitations of black holes, and noted that the frequency of the emitted radiation carried with it key information which could be used to determine the mass of the invisible black hole. These issues are still at the heart of current research three decades later.

Today, the technology to study these questions has become even more formidable, requiring large groups of researchers to work hard at developing computer codes to run on the massively parallel supercomputers of today and tomorrow. This has caused gravitational theory to enter into the realm of “big science” already familiar to experimental physics, with large, geographically distributed collaborations of scientists engaged on work on expensive, remote, central facilities. The goal of this modern work is to understand the full details of black hole collisions, the fundamental two-body problem for this field. Recent developments in this area are very encouraging, but it may well take another three decades until all the riches of this subject are mined.

In this paper, we will present all the gory details of how the best current methods in computational gravitation can be forged into a single tool to attack this crucial problem, one which is currently beyond our grasp, but perhaps not out of our reach.

2. Introduction

Although Einstein’s field equations for gravitation have been known for the past 80 years, their complexity has frustrated attempts to extract the deep intellectual content hidden beneath intractable mathematics. The only tool with potential for the study of the general dynamics of time-dependent, strongly nonlinear gravitational fields appears to be computer simulation. Over the past two decades, two alternate approaches to formulating the specification and evolution of initial data for complex physical problems have emerged. The Cauchy (also known as the ADM or “3 + 1”) approach foliates spacetime with spacelike hypersurfaces. Alternatively, the characteristic approach uses a foliation of null hypersurfaces.

Each scheme has its own different and complementary strengths and weaknesses. Cauchy evolution is more highly developed and has demonstrated good ability to handle relativistic matter and strong fields. However,
it is limited to use in a finite region of spacetime, and so it introduces an outer boundary where an artificial boundary condition must be specified. Characteristic evolution allows the compactification of the entire spacetime, and the incorporation of future null infinity within a finite computational grid. However, in turn, it suffers from complications due to gravitational fields causing focusing of the light rays. The resultant caustics of the null cones lead to coordinate singularities. At present, the unification of both of these methods [4] appears to offer the best chance for attacking the fundamental two-body problem of modern theoretical gravitation: the collision of two black holes.

The basic methodology of the new computational approach called \textit{Cauchy-characteristic matching (CCM)}, utilizes Cauchy evolution within a prescribed world-tube, but replaces the need for an outer boundary condition by matching onto a characteristic evolution in the exterior to this world-tube, reaching all the way out to future null infinity. The advantages of this approach are: (1) Accurate waveform and polarization properties can be computed at null infinity; (2) Elimination of the unphysical outgoing radiation condition as an outer boundary condition on the Cauchy problem, and with it all accompanying contamination from spurious back-reflections, consequently helping to clarify the Cauchy initial value problem. Instead, the matching approach incorporates exactly all physical backscattering from true nonlinearities; (3) Production of a global solution for the spacetime; (4) Computational efficiency in terms of both the grid domain and algorithm. A detailed assessment of these advantages is given in Sec. 3.

The main modules of the matching algorithm are:

\begin{itemize}
\item The outer boundary module which sets the grid structures.
\item The extraction module whose input is Cauchy grid data in the neighborhood of the world-tube and whose output is the inner boundary data for the exterior characteristic evolution.
\item The injection module which completes the interface by using the exterior characteristic evolution to supply the outer Cauchy boundary condition, so that no artificial boundary condition is necessary.
\end{itemize}

Details of the Cauchy and characteristic codes have been presented elsewhere. In this paper, we present only those features necessary to discuss the matching problem.

3. Advantages of Cauchy-characteristic matching (CCM)

There are a number of places where errors can arise in a pure Cauchy computation. The key advantage of CCM is that there is tight control over the errors, which leads to computational efficiency in the following sense. For a given target error $\varepsilon$, what is the amount of computation required for
CCM (denoted by $A_{CCM}$) compared to that required for a pure Cauchy calculation (denoted by $A_{WE}$)? It will be shown that $A_{CCM}/A_{WE} \to O$ as $\varepsilon \to O$, so that in the limit of high accuracy CCM is by far the most efficient method.

In CCM a “3 + 1” interior Cauchy evolution is matched to an exterior characteristic evolution at a world-tube of constant radius $R$. The important point is that the characteristic evolution can be rigorously compactified, so that the whole spacetime to future null infinity may be represented on a finite grid. From a numerical point of view this means that the only error made in a calculation of the gravitational radiation at infinity is that due to the finite discretization $h$; for second-order algorithms this error is $O(h^2)$. The value of the matching radius $R$ is important, and it will turn out that for efficiency it should be as small as possible. The difficulty is that if $R$ is too small then caustics may form. Note however that the smallest value of $R$ that avoids caustics is determined by the physics of the problem, and is not affected by either the discretization $h$ or the numerical method.

On the other hand, the standard approach is to make an estimate of the gravitational radiation solely from the data calculated in a pure Cauchy evolution. The simplest method would be to use the raw data, but that approach is too crude because it mixes gauge effects with the physics. Thus a substantial amount of work has gone into methods to factor out the gauge effects and to produce an estimate of the gravitational field at null infinity from its behavior within the domain of the Cauchy computation [5, 6, 7]. We will call this method waveform extraction, or WE. The computation is performed in a domain $D$, whose spatial cross-section is finite and is normally spherical or cubic. Waveform extraction is computed on a world-tube $\Gamma$, which is strictly in the interior of $D$, and which has a spatial cross-section that is spherical and of radius $r_E$. While WE is a substantial improvement on the crude approach, it has limitations. Firstly, it disregards the effect, between $\Gamma$ and null infinity, of the nonlinear terms in the Einstein equations; the resulting error will be estimated below. Secondly, there is an error, that appears as spurious wave reflections, due to the inexact boundary condition that has to be imposed at $\partial D$. However, we do not estimate this error because it is difficult to do so for the general case; and also because it is in principle possible to avoid it by using an exact artificial boundary condition (at a significant computational cost).

The key difference between CCM and WE is in the treatment of the nonlinear terms between $\Gamma$ and future null infinity. WE ignores these terms, and this is an inherent limitation of a perturbative method (even if it is possible to extend WE beyond linear order, there would necessarily be a cutoff at some finite order). Thus our strategy for comparing the computational efficiency of CCM and WE will be to find the error introduced into WE from
ignoring the nonlinear terms; and then to find the amount of computation needed to control this error.

3.1. ERROR ESTIMATE IN WE

As discussed earlier, ignoring the nonlinear terms between $\Gamma$ (at $r = r_E$) and null infinity introduces an error, which we estimate using characteristic methods. The Bondi-Sachs metric is

$$ds^2 = -\left(\frac{e^{2\beta}V}{r} - r^2 h_{AB}U^A U^B\right)du^2 - 2e^{2\beta} dudr - 2r^2 h_{AB} U^B dudx^A + r^2 h_{AB} dx^A dx^B,$$  

(1)

where $A, B = 2, 3$ and $h_{AB}$ is a spherical metric that is completely described by one complex function $J$. The initial data required on a null cone $u = constant$ is $J$, and the hypersurface equations $R_{1\alpha} = 0$ then form a hierarchy from which $\beta$, $U^A$ and $W \equiv (V - r)/r^2$ are found [11]. The evolution equation $R_{AB} h^{AB} = 0$ [11] is

$$2(rJ)_{,ur} = L_J + N_J$$  

(2)

where $L_J$ represents the linear part and $N_J$ the nonlinear part.

The order of magnitude of various terms can be expressed in terms of a function $c(u, x^A)$ (whose time derivative $c_u$ is the news function); note that $c$ is not a small quantity. The expressions are

$$J = O\left(\frac{c}{r}\right), \beta = O\left(\frac{c^2}{r^2}\right), U^A = O\left(\frac{c}{r^2}\right), W = O\left(\frac{c^2}{r^2}\right).$$  

(3)

These estimates are obtained from the hypersurface equations, and assume that the background geometry is Minkowskian. Should this not be the case then constants of order unity would be added, and the effect of this would be to amend (2) by adding terms to $L_J$ so that it represents wave propagation on a non-Minkowskian background. However, the order of magnitude of terms in $N_J$ would not be affected. It is straightforward to confirm that $N_J$ involves terms of order

$$O\left(\frac{c^2}{r^3}\right).$$  

(4)

WE estimates the news at future null infinity from data at $r = r_E$, and could be made exact if $N_J$ were zero. Thus the error introduced by ignoring $N_J$ is

$$\varepsilon(c, u) \equiv (c, u)_{exact} - (c, u)_{WE} = \int_{r_E}^{\infty} O\left(\frac{c^2}{r^3}\right) dr = O\left(\frac{c^2}{r_E^2}\right).$$  

(5)
This would be the unavoidable linearization error in WE were it imple-
mented as an “exact” artificial boundary condition by using global tech-
niques, such as the difference potential method, to eliminate back reflect-
ation at the boundary [8]. However, this is computationally expensive [9]
and has not even been attempted in general relativity. The performance of
WE continues to improve but the additional error due to back reflection
remains [10].

3.2. COMPUTATIONAL EFFICIENCY

A numerical calculation of the emission of gravitational radiation using a
CCM algorithm is expected to be second-order convergent, so that after a
fixed time interval the error is:

$$\varepsilon = O(h^2) \simeq k_1 h^2,$$  \hspace{1cm} (6)

where \( h \) is the discretization length. On the other hand, the same calculation
using WE must allow for the error found in (5), and therefore after the same
fixed time interval there will be an error of:

$$\varepsilon = O(h^2, r_E^{-2}) \simeq \max(k_2 h^2, \frac{k_3}{r_E^2}).$$  \hspace{1cm} (7)

We now estimate the amount of computation required for a given desired
accuracy. We make one important assumption:

− The computation involved in matching, and in waveform extract,
is an order of magnitude smaller than the computation involved in
evolution, and is ignored.

For the sake of transparency we also make some simplifying assumptions; if
not true there would be some extra constants of order unity in the formulas
below, but the qualitative conclusions would not be affected.

1. The amount of computation per grid point per time-step, \( a \), is the
same for the Cauchy and characteristic algorithms.
2. The constants \( k_1, k_2 \) in the equations above are approximately equal
and will be written as \( k \).
3. In CCM, the numbers of Cauchy and characteristic grid-points are the
same; thus the total number of grid points per time-step is:

$$\frac{8\pi R^3}{3h^3}. \hspace{1cm} (8)$$

4. In WE, the number of grid points in \( D \) is twice the number contained
in \( \Gamma \); thus the total number of grid points per time-step is

$$\frac{8\pi r_E^3}{3h^3}. \hspace{1cm} (9)$$
It follows that the total amount of computation $A$ (i.e., number of floating-point operations) required for the two methods is:

$$A_{CCM} = \frac{8\pi R^3 a}{3h^4}, \quad A_{WE} = \frac{8\pi r_E^3 a}{3h^4}. \quad (10)$$

Thus $R > r_E$ or $R < r_E$ determines which method requires the least amount of computation. Because of the assumptions (1) to (4) this criterion is not exact but only approximate.

As stated earlier, in a given physical situation the minimum allowed value of $R$ is determined by the physics. However, $r_E$ is determined by the target error (equation (7)); and there is also a minimum value determined by the condition that the nonlinearities must be sufficiently weak for a perturbative expansion to be possible. Thus, in a loose sense, the minimum value of $r_E$ is expected to be related to the minimum value of $R$. It follows that the computational efficiency of a CCM algorithm is never expected to be significantly worse than that of a WE algorithm.

If high accuracy is required, the need for computational efficiency always favors CCM. More precisely, for a given desired error $\varepsilon$, equations (6) and (7), and assumption (2), imply:

$$h = \sqrt{\varepsilon/k}, \quad r_E = \sqrt{k_3/\varepsilon}. \quad (11)$$

Thus, substituting equation (11) into equation (10),

$$A_{CCM} = \frac{8\pi R^3 a k^2}{3\varepsilon^2}, \quad A_{WE} = \frac{8\pi ak^2 k_3^{3/2}}{3\varepsilon^{7/2}}, \quad (12)$$

so that

$$\frac{A_{CCM}}{A_{WE}} = \frac{R^3 \varepsilon^{3/2}}{k_3^{3/2}} \to 0 \text{ as } \varepsilon \to 0. \quad (13)$$

This is the crucial result, that the computational intensity of CCM relative to that of WE goes to zero as the desired error $\varepsilon$ goes to zero.

4. Extraction

We describe a procedure by which information about the 4-geometry on the neighborhood of a world-tube $\Gamma$, obtained during a 3 + 1 simulation of Einstein’s equations, is used to extract boundary data appropriate for an exterior characteristic formulation. A numerical implementation of this characteristic formulation [12], is then used to propagate the gravitational signal to null infinity, where the radiation patterns are calculated. The process we describe here is non-perturbative, and to make it as portable as
possible, it assumes only that the 3+1 simulation can provide the 3-metric, the lapse and the shift by interpolation to a set of prescribed points.

We start by describing the world-tube $\Gamma$ in Sec. 4.1, we explain what information needs to be provided by the 3+1 simulation around the world-tube in Sec. 4.2, giving details of the transformation to null coordinates in Sec. 4.3, and the expression for the Bondi metric in Sec. 4.5. This provides the boundary data needed to start up the characteristic code in Sec. 4.6. The characteristic code which takes this boundary information and calculates the waveforms is described in detail in [12].

4.1. PARAMETRIZATION OF THE WORLD-TUBE

The notation and formalism are based on Misner, Thorne and Wheeler [13]. Greek indices range from 1 to 4, Latin indices range from 1 to 3, and upper case Latin indices refer to coordinates on the sphere and range from 2 to 3.

The intersections $S_t$ of the world-tube with the space-like slices $\Sigma_t$ of the Cauchy foliation are topologically spherical, and they can be parametrized by labels $\tilde{y}^A$, $A = [2,3]$ on the sphere. The intersections themselves are labeled by the time coordinate of the Cauchy foliation, $x^4 = t$. Future oriented null cones emanating from the world-tube are parametrized by the labels on the sphere $\tilde{y}^A$ and an affine parameter $\lambda$ along the radial direction, with $\lambda = 0$ on the world-tube. With the identifications $\tilde{y}^1 = \lambda$ and retarded time $\tilde{y}^4 = u = t$, we define a null coordinate system $\tilde{y}^\alpha = (\tilde{y}^1, \tilde{y}^A, \tilde{y}^4)$. We will later introduce a second null coordinate system $y^\alpha = (y^1, y^A, y^4)$, where $y^1 = r$, $r$ being a surface area coordinate, and $y^A = \tilde{y}^A$, $y^4 = \tilde{y}^4$.

Following [14], we cover the unit sphere with two stereographic coordinate patches, centered around the North and South poles, respectively, where the stereographic coordinate is related to the usual spherical polar coordinates $(\theta, \phi)$ by

$$\xi_{\text{North}} = \left\{ \begin{array}{ll} \sqrt{\frac{1 - \cos \theta}{1 + \cos \theta}} e^{i\phi}, & \text{if} \quad \xi = \tilde{y}^2 + i\tilde{y}^3 = q + ip; \\ \sqrt{\frac{1 + \cos \theta}{1 - \cos \theta}} e^{-i\phi}, & \text{if} \quad \xi = \tilde{y}^2 - i\tilde{y}^3 = q - ip. \end{array} \right.$$ (14)

Let $\tilde{y}^A \equiv (q, p)$, for $A = [2,3]$, label the points of a stereographic coordinate patch. We adopt as these labels the real and imaginary part of the stereographic coordinate, i.e. for $\xi = \tilde{y}^2 + i\tilde{y}^3 = q + ip$.

For the computational implementation of the procedure we are describing, we introduce a discrete representation of these coordinate patches

$$\tilde{y}_i^2 = -1 + (i - 3)\Delta, \quad \tilde{y}_j^3 = -1 + (j - 3)\Delta,$$ (15)

where the computational spatial grid indices $i, j, k$ run from 1 to $N$ and $\Delta = 2/(N - 5)$, $N$ is the stereographic grid size and $\Delta$ the stereographic grid spacing.
On each patch, we introduce complex null vectors on the sphere \( q^A = (P/2)(\delta^A_2 + i\delta^A_3) \), where \( P = 1 + \xi \bar{\xi} \). The vectors \( q_A, \bar{q}_A \) define a metric on the unit sphere

\[
q_{AB} = \frac{1}{2}(q_A \bar{q}_B + \bar{q}_A q_B) = \frac{4}{P^2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}
\]  

(16)

with determinant \( \det(q_{AB}) = 16/P^4 \). The co-vector \( \bar{q}_A \) satisfies the orthogonality condition \( \bar{q}_A q^A = 2 \), and has components \( q_A = (2/P)(\delta^2_A + i\delta^3_A) \).

Given Cartesian coordinates \( x^i = (x, y, z) \) on a space-like slice \( \Sigma_t \), the intersection \( S_t \) of the world-tube \( \Gamma \) with \( \Sigma_t \) is described parametrically by three functions of the \( \tilde{y}^A, x^{(0)i} = f^i(\tilde{y}^A) \). In the following, we will fix the location of the world-tube by choosing these functions (in stereographic coordinates) as:

\[
\begin{align*}
    f^x(\tilde{y}^A) &= 2R \left( \frac{\Re(\xi)}{1 + \xi \bar{\xi}} \right) \\
    f^y(\tilde{y}^A) &= \pm 2R \left( \frac{\Im(\xi)}{1 + \xi \bar{\xi}} \right) \\
    f^z(\tilde{y}^A) &= \pm R \left( \frac{1 - \xi \bar{\xi}}{1 + \xi \bar{\xi}} \right)
\end{align*}
\]  

(17)

where the positive (negative) sign corresponds to the north (south) patch. This defines a canonical spherical section \( S_t \) of radius \( R \) in Minkowski-space. Note that this provides a prescription for locating the world-tube which is time-independent.

Given two 3-dimensional quantities \( v^i \) and \( w^i \), we introduce their Euclidean inner product \( (v \cdot w) = \delta_{ij} v^i w^j \). The stereographic coordinates of points on the surface of the 3-sphere with Cartesian coordinates \( x^i = (x, y, z) \) can then be represented by \( y^A(x^i) = (q, p) \), with

\[
q(x^i) = \frac{x}{\hat{r} \pm z}, \quad p(x^i) = \pm \frac{y}{\hat{r} \pm z}
\]  

(18)

on the north (+) and south (−) patches, where

\[
\hat{r}^2 = (x \cdot x).
\]  

(19)

Note that the stereographic coordinates are invariant under a change of scale, \( y^A(x^i) = y^A(cx^i) \).

The Euclidean radius of the world-tube with Cartesian coordinates \( x^{(0)i} \) is given by:

\[
R^2 = (x^{(0)} \cdot x^{(0)}).
\]  

(20)
This equation provides a particularly simple alternate definition of the choice of world-tube using Cartesian coordinates. This definition also holds for each instant of Cartesian time.

4.2. 4-D GEOMETRY AROUND THE WORLD-TUBE

The 4-d geometry around the world-tube is fully specified by the 4-d metric and its derivatives (alternatively, by the metric and the metric connection). They determine the unit normal \( n^\alpha \) to the \( t = \text{constant} \) slices, and given the parametrization of the world-tube, the (outward pointing) normal \( s^\alpha \) to the world-tube. They also determine the generator of the outgoing null radial geodesics through the world-tube, which in turn completes the specification of the coordinate transformation \( x^\alpha \rightarrow \tilde{y}^\alpha \) in a neighborhood of the world-tube.

In practice, the necessary information is not available at the discrete set of points on the world-tube specified by Eqs. (14) and (17) where \( \xi_{ij} = \tilde{y}_1^2 + i\tilde{y}_3^3 \) as given in Eq. (15). However, the required variables are known on the points of the computational grid used in the simulation, a Cartesian grid \((x_i, y_j, z_k)\), from which we interpolate them to the world-tube points to second order accuracy.

For a standard \(3+1\) simulation [15], the variables that we need to interpolate are the 3-d metric \( g_{ij} \), the lapse \( \alpha \) and the shift \( \beta^i \). Their spatial derivatives are also interpolated. Their values at the world-tube points are stored for a number of time levels, and the time derivatives of the 3-metric, lapse and shift at the world-tube are computed by finite-differencing between these time levels.

Using all these values we can compute the 4-metric \( g_{\mu\nu} \), and its first derivatives \( g_{\mu\nu,\sigma} \), using the following relations:

\[
\begin{align*}
g_{it} &= g_{ij}\beta^j \\
g_{tt} &= -\alpha^2 + g_{it}\beta^i \\
g_{it,\mu} &= g_{ij,\mu}\beta^j + g_{ij}\beta^j_{,\mu} \\
g_{tt,\mu} &= -2\alpha\alpha_{,\mu} + g_{ij,\mu}\beta^i\beta^j + 2g_{ij}\beta^i\beta^j_{,\mu}.
\end{align*}
\] (21)

The unit normal \( n^\mu \) to the hypersurface \( \Sigma_t \) is determined from the lapse and shift

\[
n^\mu = \frac{1}{\alpha} \left( 1, -\beta^i \right). \tag{22}
\]

Let \( s^\alpha = (s^i, 0) \) be the outward pointing unit normal to the section \( S_t \) of the world-tube at time \( t^n \). By construction, \( s^i \) lies in the slice \( \Sigma_t \), and it is
known given the two vectors $\partial_{\tilde{y}^2}$, $\partial_{\tilde{y}^3}$ in $S_t$, defined by the parametrization of the world-tube $x^i(\tilde{y}^A)$

\[
q^i = \frac{\partial x^i}{\partial \tilde{y}^2}, \quad p^i = \frac{\partial x^i}{\partial \tilde{y}^3}.
\]

These may be obtained analytically from Eq. (17), the equation for the world tube. Antisymmetrizing $q^i$ and $p^i$, we obtain the spatial components of the normal 1-form $\sigma_i$ and its norm $\sigma$

\[
\sigma_i = \epsilon_{ijk} q^j p^k, \quad \sigma = \sqrt{g^{ij} \sigma_i \sigma_j}
\]

from which $s^i$ is obtained by raising $\sigma_i$ with the contravariant 3-metric $g^{ij}$ on the slice $\Sigma_t$ and dividing by the norm $\sigma$, yielding

\[
s^i = g^{ij} \frac{\sigma_j}{\sigma}.
\]

The generators $\ell^\alpha$ of the outgoing null cone $C_t$ through $S_t$ are given on the world-tube by

\[
\ell^\alpha = \frac{n^\alpha + s^\alpha}{\alpha - g_{ij} \beta^i s^j}
\]

which is normalized so that $\ell^\alpha t_\alpha = -1$, where $t^\alpha = \alpha n^\alpha + \beta^\alpha$ is the Cauchy evolution vector.

The equations in this section show explicitly how to use the output data from the Cauchy simulation to completely reconstruct the full 4-geometry of the spacetime, as well as other important geometrical objects of interest, in the neighborhood of the world-tube $\Gamma$. This is all described in this section within the Cartesian coordinate system used by the 3+1 computation, and holds to the second-order accuracy assumed for this computation. In the next three sections, we will demonstrate how to use this information to redescribe the same geometry in another coordinate system, the Bondi coordinates needed for characteristic simulations. There is nothing in these sections that goes beyond the elementary concepts of defining coordinate systems and transforming tensors under a change of coordinates. Nevertheless, it is quite instructive to see just how much work lies hidden beneath the clever notation used by theorists.

4.3. COORDINATE TRANSFORMATION

In this section we build the coordinate transformation between the 3 + 1 Cartesian coordinates $x^\alpha$ and the (null) affine coordinates $\tilde{y}^\alpha$. We will need this in the neighborhood of the world-tube, not just at a point on the tube, in order to easily pass information back and forth between the
Cauchy and characteristic computer codes in the overlap region near the world-tube. In Sec. 4.4, we will transform the metric to affine coordinates. Finally, in Sec. 4.5, we will complete the transformation from affine to Bondi coordinates.

The motivation for this indirect route to the Bondi coordinate frame deserves some comment. Both affine coordinates $\tilde{y}^\alpha$ and Bondi coordinates $y^\alpha$ utilize null hypersurfaces for foliations. Calculating these directly would require the numerical solution of a nonlinear partial differential equation (the eikonal equation). A much simpler, but physically equivalent, approach is to instead solve the null geodesic equation in Cartesian coordinates, in order to find the rays $x^\mu(\lambda)$ generating the required null hypersurfaces. Secondly, we must introduce the intermediary of the affine radial coordinate $\lambda$ rather than the Bondi surface area coordinate $r$, since the latter is actually unknown until the angular coordinates are defined. As shown below, it is only after the null rays have been found that we are able to proceed with the orderly introduction of angular coordinates $\tilde{y}^A$ in the exterior of the world-tube. Finally, null geodesics can be analytically constructed trivially in terms of $\lambda$, whereas even when we have defined the surface area coordinate $r$, solution of the null geodesics equation requires the numerical solution of an ordinary differential equation. With this rationale complete, we will now proceed to carry out the coordinate definitions and transform the metric.

By inspection, $x^\alpha(\lambda)$, the solution to the geodesic equation relating $x^\alpha$ to $\tilde{y}^\alpha$ off the world-tube is:

$$x^\alpha = x^{(0)}{}^\alpha + \ell^{(0)}{}^\alpha \lambda + O(\lambda^2).$$  \hspace{1cm} (27)

This expression determines $x^\alpha(\lambda)$ to $O(\lambda^2)$, given the coefficients

$$x^{(0)}{}^\alpha = x^\alpha |_\Gamma \quad \text{and} \quad \ell^{(0)}{}^\alpha = x_\lambda |_\Gamma$$  \hspace{1cm} (28)

that is, given the coordinates of the points and the generators of the null cone through the world-tube section $S_t$. For completeness, we repeat the remaining coordinate relations defined in Sec. 4.1. Along each outgoing null geodesic emerging from $S_t$, angular and time coordinates are defined by setting their values to be constant along the rays, and equal to their values on the world-tube

$$\tilde{y}^A = y^A |_\Gamma \quad \text{and} \quad \tilde{y}^4 \equiv \tilde{u} = t.$$  \hspace{1cm} (29)

Given the coordinate transformation $x^\mu = x^\mu(\tilde{y}^\alpha)$, we obtain the metric in null affine coordinates $\tilde{\eta}_{\alpha\beta}$ by

$$\tilde{\eta}_{\alpha\beta} = \frac{\partial x^\mu}{\partial \tilde{y}^\alpha} \frac{\partial x^\nu}{\partial \tilde{y}^\beta} g_{\mu\nu}.$$  \hspace{1cm} (30)
The Jacobian of the coordinate transformation is viewed as a series expansion in the affine parameter $\lambda$ for each point on the world-tube. Furthermore, we may omit the $\lambda$ derivatives of the $x^\mu$, i.e. the $x^\mu_{,\lambda}$ are not needed because the radial coordinate $\lambda$ is an affine parameter of the null geodesics, hence the $\tilde{\eta}_{\lambda\bar{\lambda}}$ components of the null metric are fixed:

$$\tilde{\eta}_{\lambda\lambda} = \tilde{\eta}_{\lambda\bar{A}} = 0, \quad \tilde{\eta}_{\lambda\bar{u}} = -1,$$

(31)

(This follows from the conditions $s^\alpha n_\alpha = 0$, $\ell^\alpha \ell_\alpha = 0$, $s^\alpha s_\alpha = 1$, $n^\alpha n_\alpha = -1$ and $t^\alpha \ell_\alpha = -1$). In other words, $\tilde{\eta}_{\lambda\bar{\lambda}}$ contains six independent metric functions. The relevant part of the coordinate transformation is then

$$x^\mu_{,\tilde{\alpha}} = \frac{\partial x^\mu}{\partial \tilde{y}^\alpha} = x^{(0)\mu}_{,\tilde{\alpha}} + x^{(1)\mu}_{,\tilde{\alpha}} \lambda + O(\lambda^2), \quad x^{(1)\mu}_{,\tilde{\alpha}} \equiv \ell^{(0)\mu}_{,\tilde{\alpha}}, \quad \text{for} \quad \tilde{\alpha} = (\tilde{A}, \tilde{u}).$$

(32)

Because the specification of the world-tube is time-independent, and the slices $S_t$ of the world-tube are by construction at $t = constant$, only the angular derivatives of the $x^{(0)i}$ for $i = 1, 2, 3$ survive, i.e. the $O(\lambda^0)$ part of the Jacobian is given by the condition $\partial t / \partial \tilde{u} \mid_\Gamma = 1$, and by the relations

$$x^{(0)i}_{,\tilde{A}} = \frac{\partial f^i(\tilde{y}^B)}{\partial \tilde{y}^A},$$

(33)

which can be evaluated from the analytic expressions Eq. (17).

To evaluate the $O(\lambda)$ part of the Jacobian, we note that

$$x^\mu_{,\lambda \tilde{A}} \equiv \ell^{\mu}_{,\lambda \tilde{A}}, \quad x^\mu_{,\lambda \tilde{u}} = \ell^{\mu}_{,\lambda \tilde{u}}$$

(34)

We will spend the remainder of this section evaluating these terms. To proceed, we see from Eq. (26) that this will require derivatives of $n^\mu$ and $s^i$. For the simple case of geodesic slicing, $\alpha = 1$, $\beta^i = 0$, the derivatives of the normal $n^\mu$ vanish, and the transformation is contained purely in the derivatives of $s^i$. In general, the angular derivatives of $n^\mu$ at $\lambda = constant$ can be computed in terms of spatial 3+1 derivatives of the lapse and shift, transformed with the $O(\lambda^0)$ Jacobian, i.e.

$$n^\mu_{,\tilde{A}} = n^\mu_{,\tilde{J}} x^J_{,\tilde{A}}$$

(35)

The 3+1 derivatives are given by

$$n^i_{,j} = \frac{1}{\alpha^2}(\alpha_{,j} \beta^i - \alpha \beta^i_{,j})$$

$$n^t_{,j} = -\frac{1}{\alpha^2} \alpha_{,j}.$$

(36)
The retarded time derivative $\partial_{\tilde{u}}$ at $\lambda = constant$ is simply the $3 + 1$ time derivative $\partial_t$, therefore $n^t_{\tilde{u}} = n^t_t$, where

\[
\begin{align*}
n^t_t &= \frac{1}{\alpha^2} \left( \alpha_{,t} \beta^t - \alpha_{,t} \beta^t \right), \\
n^t_{,t} &= -\frac{1}{\alpha^2} \alpha_{,t}.
\end{align*}
\]  
(37)

From Eq. (25), and since the $\sigma_k$ are time-independent, the time derivative of $s^i$ is given by

\[
\begin{align*}
s^i_{,t} &= g^{ik}_{t, \sigma} \sigma_k - \frac{g^{ik} \sigma_k \sigma \sigma \sigma^{,t}}{\sigma^2} = -g^{im} g^{kn} g_{mn, t} \frac{\sigma_k}{\sigma} - s^i \frac{\sigma \sigma \sigma \sigma}{\sigma} \\
&= -g^{im} g_{mn, t} s^n - s^i \frac{\sigma \sigma \sigma \sigma}{\sigma}
\end{align*}
\]  
(38)

where the time derivative of $\sigma$ can be calculated from

\[
2 \sigma_{,t} = \left( \sigma^2 \right)_{,t} = g^{kl}_{t, \sigma} \sigma_k \sigma_l = -g^{km} g^{ln} g_{mn, t} = -s^m s^n g_{mn, t} \sigma^2,
\]
(39)

with the resulting expression

\[
s^i_{,t} = \left( -g^{im} + s \frac{1}{2} s^n \right) g_{mn, t} s^n.
\]
(40)

Similarly, it follows from Eq. (25) that

\[
\begin{align*}
s^j_{,A} &= g^{jk}_{,A} x^j_{,A} \frac{\sigma_k}{\sigma} + g^{jk} \sigma_k \sigma_{,A} - \frac{g^{jk} \sigma_k \sigma_{,A}}{\sigma^2} \\
&= -g^{im} g^{km} g_{mn, j} x^j_{,A} \frac{\sigma_k}{\sigma} + g^{jk} \sigma_k \sigma_{,A} - s^i \frac{\sigma \sigma \sigma \sigma}{\sigma}
\end{align*}
\]  
(41)

where the $\sigma_k_{,A}$ are obtained from the analytic expressions Eq. (17), and $\sigma_{,A}$ from

\[
\begin{align*}
2 \sigma_{,A} &= \left( \sigma^2 \right)_{,A} = \left( g^{kl} \sigma_k \sigma_l \right)_{,A} = g^{kl}_{,A} x^j_{,A} \sigma_k \sigma_l + 2 g^{kl} \sigma_l \sigma_{k,\tilde{A}} \\
&= -g^{km} g^{ln} g_{mn, j} x^j_{,A} \sigma_k \sigma_l + 2 g^{kl} \sigma_l \sigma_{k,\tilde{A}} \\
&= -s^m s^n g_{mn, j} x^j_{,A} \sigma^2 + 2 s^k \sigma \sigma_{k,\tilde{A}}
\end{align*}
\]  
(42)

Collecting Eqs. (41) and (42), we arrive at the angular derivatives of the normal to the world-tube.
Cauchy-characteristic matching

\[ s^i_{\cdot A} = -g^{in} s^m g_{mn,j} x^j_{\cdot A} + g^{ik} \frac{\sigma_{k \cdot A}}{\sigma} + s^i \left( \frac{1}{2} s^m s^n g_{mn,j} x^j_{\cdot A} - s^k \frac{\sigma_{k \cdot A}}{\sigma} \right) \]

\[ = \left( g^{in} - s^i s^n \right) \frac{\sigma_{n \cdot A}}{\sigma} + \left( -g^{in} + \frac{1}{2} s^i s^n \right) s^m g_{mn,j} x^j_{\cdot A}. \] (43)

4.4. NULL METRIC \( \tilde{\eta}_{\alpha \beta} \)

Given the 4-metric and its Cartesian derivatives at the world-tube, we can calculate its derivative with respect to the affine parameter \( \lambda \) according to

\[ g_{\alpha \beta, \lambda}^{(0)} |_{\Gamma} = g_{\alpha \beta, \mu}^{(0)} \ell_{\mu}^{(0)} \] (44)

Having obtained the relevant parts of the coordinate transformation \( \tilde{g}^\alpha \to x^\alpha \), Eqs. (34), (35), (36), (37), (40), and (43), and given the metric and its \( \lambda \) derivative as per Eq. (44), we can expand the null metric as follows

\[ \tilde{\eta}_{\alpha \beta} = \tilde{\eta}_{\alpha \beta}^{(0)} + \tilde{\eta}_{\alpha \beta, \lambda} \lambda + O(\lambda^2), \] (45)

where the coefficients are given by

\[ \tilde{\eta}_{\alpha \alpha}^{(0)} = g_{tt} |_{\Gamma} \]
\[ \tilde{\eta}_{\alpha A}^{(0)} = x^i_{\cdot A} g_{tt} |_{\Gamma} \]
\[ \tilde{\eta}_{AB}^{(0)} = x^i_{\cdot A} x^j_{\cdot B} g_{ij} |_{\Gamma} \] (46)

and, for the \( \lambda \) derivative

\[ \tilde{\eta}_{\alpha \alpha, \lambda} = \left[ g_{tt, \lambda} + 2 \ell^\mu_{\alpha} g_{\mu \lambda} \right] |_{\Gamma} + O(\lambda) \]
\[ \tilde{\eta}_{\alpha A, \lambda} = \left[ x^k_{\cdot A} \left( \ell^\mu_{\alpha} g_{k \lambda} + g_{k t, \lambda} \right) + \ell^k_{\cdot A} g_{k t} + \ell^t_{\cdot A} g_{tt} \right] |_{\Gamma} + O(\lambda), \]
\[ \tilde{\eta}_{AB, \lambda} = \left[ x^k_{\cdot A} x^l_{\cdot B} g_{kl, \lambda} + \left( \ell^\mu_{\cdot A} x^l_{\cdot B} + \ell^\mu_{\cdot B} x^l_{\cdot A} \right) g_{\mu \lambda} \right] |_{\Gamma} + O(\lambda). \] (47)

The remaining components are fixed by Eq. (31).

It is worthwhile to discuss a subtlety in the rationale underlying the computational strategy used here. The purpose of carrying out an expansion in \( \lambda \) is to enable us to give the metric variables in a small region off the world-tube, i.e. at points of the grid used to discretize the null equations. This method is an alternative to the more obvious and straightforward
strategy of interpolation to determine metric values at needed points on the null computational grid. At first glance, it might appear a more cumbersome way to proceed, due to the necessity of analytic calculation of the derivative of the metric on the world tube to determine coefficients needed for the metric expansion in powers of $\lambda$. On the contrary, however, this trick allows a major simplification in computer implementation. It allows us to use a null code which does not require any special implementation at the irregular boundary defined by the world-tube, and it automatically ensures continuity of the metric and the extrinsic curvature at the world-tube. The obvious alternative of a brute-force interpolation approach would require a full 4-dimensional evaluation with quite complicated logic, since it would lie at the edge of both the Cauchy and null computational grids. Instead, the $\lambda$ expansion reduces the complexity by one dimension, allowing for much easier numerical implementation.

We also need to compute the contravariant null metric, $\tilde{\eta}^{\alpha\beta}$, which we similarly consider as an expansion in powers of $\lambda$,

$$\tilde{\eta}^{\mu\nu} = \tilde{\eta}^{(0)}_{\mu\nu} + \tilde{\eta}^{(0)}_{\mu\lambda} \lambda + O(\lambda^2),$$

(48)

with coefficients given by

$$\tilde{\eta}^{(0)}_{\mu\alpha} \tilde{\eta}^{(0)}_{\alpha\nu} = \delta_\nu^\mu, \quad \tilde{\eta}^{\mu\lambda}_{\lambda\lambda} = -\tilde{\eta}^{\mu\lambda}_{\lambda\nu} \tilde{\eta}^{\nu\lambda}_{\alpha\beta,\lambda}.$$  

(49)

It follows from Eq. (31) that the following components of the contravariant null metric in the $\tilde{y}^\alpha$ coordinates are fixed

$$\tilde{\eta}^{\lambda\tilde{u}} = -1 \quad \tilde{\eta}^{\tilde{u}A} = \tilde{\eta}^{\tilde{u}\tilde{u}} = 0,$$  

(50)

together with the following equations:

$$\tilde{\eta}^{AB} \tilde{\eta}_{BC} = \delta^A_C,$$

$$\tilde{\eta}^{\lambda A} = \tilde{\eta}^{\lambda B} \tilde{\eta}_{B\tilde{u}},$$

$$\tilde{\eta}^{\lambda\lambda} = -\tilde{\eta}_{\tilde{u}\tilde{u}} + \tilde{\eta}^{\lambda\tilde{A}} \tilde{\eta}_{\tilde{A}\tilde{u}},$$

and similarly for its $\lambda$ derivative

$$\tilde{\eta}^{AB}_{\lambda} = -\tilde{\eta}^{A\tilde{C}} \tilde{\eta}_{\tilde{B}\tilde{D}} \tilde{\eta}_{\tilde{C}\tilde{D},\lambda},$$

$$\tilde{\eta}^{\lambda\lambda}_{\lambda} = \tilde{\eta}^{\lambda\tilde{B}} \left( \tilde{\eta}_{\tilde{u}\tilde{B},\lambda} - \tilde{\eta}^{\lambda\tilde{A}} \tilde{\eta}_{\tilde{A}\tilde{B},\lambda} \right),$$

$$\tilde{\eta}^{\lambda\lambda}_{\lambda} = -\tilde{\eta}_{\tilde{u}\tilde{u},\lambda} + 2 \tilde{\eta}^{\lambda\tilde{A}} \tilde{\eta}_{\tilde{u}\tilde{A},\lambda} - \tilde{\eta}^{\lambda\tilde{A}} \tilde{\eta}^{\lambda\tilde{B}} \tilde{\eta}_{\tilde{A}\tilde{B},\lambda}.$$  

(52)
4.5. METRIC IN BONDI COORDINATES

The surface area coordinate \( r(u, \lambda, \tilde{y}^A) \) is defined by

\[
r = \left( \frac{\det(\tilde{\eta}_{\tilde{A} \tilde{B}})}{\det(q_{A\dot{B}})} \right)^{\frac{1}{4}},
\]

(53)

where, for our choice of stereographic coordinates \( \xi = q + ip \), we use \( \tilde{y}^A = (q, p) \) and \( \det(q_{A\dot{B}}) = 16/(1 + q^2 + p^2)^4 \). To carry out the coordinate transformation \( \tilde{y}^A \to y^A \) on the null metric, where \( y^A = (r, y^A, u) \), we need to know \( r, \lambda, r, \tilde{A} \) and \( r, \tilde{u} \). From Eq. (53) it follows

\[
r, \lambda = r^4 \tilde{\eta}^{\tilde{A} \tilde{B}} \eta_{\tilde{A} \tilde{B}, \lambda}.
\]

(54)

Similarly,

\[
r, \hat{C} = r^4 \left( \tilde{\eta}^{\tilde{A} \tilde{B}} \eta_{\tilde{A} \tilde{B}, \hat{C}} - \frac{\det(q_{\tilde{A} \tilde{B}})}{\det(q_{A\dot{B}})} \tilde{C} \right),
\]

(55)

where

\[
\frac{\det(q_{\tilde{A} \tilde{B}})}{\det(q_{A\dot{B}})} \tilde{C} = -\frac{8}{1 + q^2 + p^2} \tilde{y}^\hat{C}
\]

\[
\tilde{\eta}^{\tilde{A} \tilde{B}, \hat{C}} = \left( \tilde{x}^i_{,A} \tilde{x}^i_{,B} + x^i_{,A} x^j_{,B} \right) g_{ij} + x^i_{,A} x^j_{,B} x^k_{,C} g_{ij,k}
\]

(56)

with the \( x^i_{,A} \) given functions of \( (q, p) \). From Eqs. (53) and (46)

\[
r, \tilde{u} = r^4 \tilde{\eta}^{\tilde{A} \tilde{B}} \eta_{\tilde{A} \tilde{B}, \tilde{u}}
\]

(57)

where

\[
\tilde{\eta}^{\tilde{A} \tilde{B}, \tilde{u}} = \left[ x^j_{,A} x^j_{,B} g_{ij} \right]_{\Gamma} + O(\lambda).
\]

(58)

The null metric \( \eta^{\alpha \beta} \) in Bondi coordinates is defined on the world-tube \( \Gamma \) by

\[
\eta^{\alpha \beta} = \frac{\partial y^\alpha}{\partial \tilde{y}^\mu} \frac{\partial y^\beta}{\partial \tilde{y}^\nu} \tilde{\eta}^{\tilde{\mu} \tilde{\nu}}
\]

(59)

Note that the metric of the sphere is unchanged by this coordinate transformation, i.e. \( \eta^{AB} = \tilde{\eta}^{\tilde{A} \tilde{B}} \), so we need to compute only the elements \( \eta^{rr}, \eta^{ru} \) and \( \eta^{uA} \) on \( \Gamma \), or equivalently the metric functions \( \beta, U^A \) and \( V \). From Eq. (50),
The contravariant Bondi metric can be written in the form

$$\eta^\alpha{}^\beta = \begin{bmatrix} e^{-2\beta} \frac{V}{r} & -e^{-2\beta} U^2 & -e^{-2\beta} U^3 & -e^{-2\beta} \\ -e^{-2\beta} U^2 & r^{-2} h^{22} & r^{-2} h^{23} & 0 \\ -e^{-2\beta} U^3 & r^{-2} h^{32} & r^{-2} h^{33} & 0 \\ -e^{-2\beta} & 0 & 0 & 0 \end{bmatrix},$$

where $h_{AB}$ is a metric on the sphere of surface area $4\pi$, such that $h_{AB} h_{BC} = \delta^C_A$ and $\det(h_{AB}) = \det(q_{AB}) = q$, for $q_{AB}$ a unit sphere metric.

4.6. BONDI VARIABLES FOR STARTING UP THE NULL CODE AT THE WORLD-TUBE

The natural variables of the null formalism are certain combinations of the null metric functions, which we will give in this section. They will be expressed as an expansion in $\lambda$, as was done in the previous sections, to enable us to give these variables in a small region off the world-tube, i.e. at points of the grid used to discretize the null equations. These expressions are the main results of the extraction module.

4.6.1. The metric of the sphere $J$

Given $r$ and $r,\lambda$, and noting that

$$\eta_{AB} = \tilde{\eta}_{AB} \equiv r^2 h_{AB},$$

$$h_{AB} = \frac{1}{r^2} \eta_{AB},$$

$$h_{AB,\lambda} = \frac{1}{r^2} \left( \eta_{AB,\lambda} - \frac{2}{r} r_{\lambda} \eta_{AB} \right)$$

In terms of $q^A, \bar{q}^A$ and the metric on the unit sphere $h_{AB}$, we define the metric functions

$$J \equiv \frac{1}{2} q^A q^B h_{AB}, \quad K \equiv \frac{1}{2} q^A q^B h_{AB}, \quad K^2 = 1 + J \bar{J}. $$
It suffices to evaluate $J$, since the last relation holds for a Bondi metric. We give expressions for $J$ and $J_{\lambda}$

\[ J = \frac{1}{2r^2} q^A q^B \eta_{AB} \]

\[ J_{\lambda} = \frac{1}{2r^2} q^A q^B \eta_{AB,\lambda} - \frac{1}{r} \frac{r_{,\lambda}}{r} J \]  

(65)

Then, in the neighborhood of $\Gamma$, the metric of the sphere is explicitly given in Bondi coordinates to second-order accuracy by these last two expressions as

\[ J(y^\alpha) = J + J_{,\lambda} \lambda + O(\lambda^2). \]  

(66)

4.6.2. The “expansion factor” $\beta$

From the last of Eq. (60) we obtain the metric function $\beta$

\[ \beta = -\frac{1}{2} \log(r_{,\lambda}). \]  

(67)

We want to know also its $\lambda$-derivative, but instead of calculating $\eta^u_{\lambda}$ directly (which would involve $r_{,\lambda\lambda}$)

\[ \beta_{,\lambda} = -\frac{\eta^u_{\lambda}}{2\eta^u_{\lambda}} = -\frac{r_{,\lambda\lambda}}{2r_{,\lambda}} \]  

(68)

we obtain $\beta_{,\lambda}$ from the characteristic equation

\[ \beta_{,r} = \frac{r}{8} \left( J_{,r} \bar{J}_{,r} - (K_{,r})^2 \right) \]  

(69)

At constant angles $(q,p)$, the relation $\partial_{,\lambda} = r_{,\lambda} \partial_r$ holds, and we know from Eq. (65) $J$ and $J_{,\lambda}$ for each outgoing radial null geodesic through the world-tube, thus we can write

\[ \beta_{,\lambda} = \frac{r}{8r_{,\lambda}} \left( J_{,\lambda} \bar{J}_{,\lambda} - (K_{,\lambda})^2 \right) \]  

(70)

and from Eq. (64), it follows that

\[ K_{,\lambda} = \frac{1}{K} \Re(JJ_{,\lambda}). \]  

(71)

\[ \beta_{,\lambda} = \frac{r}{8r_{,\lambda}} \left( J_{,\lambda} \bar{J}_{,\lambda} - \frac{1}{1 + JJ} [\Re(JJ_{,\lambda})]^2 \right). \]  

(72)

Then, $\beta$ is found to second-order accuracy by:

\[ \beta(y^\alpha) = \beta + \beta_{,\lambda} \lambda + O(\lambda^2). \]  

(73)
4.6.3. The “shift” $U$

The metric function $U$ is related to the Bondi metric, Eq. (61) by

$$U \equiv U^A q_A = \frac{\eta^r}{\eta^r u} q_A = -\left(\eta^{\lambda\tilde{\lambda}} + \frac{r^\cdot B}{r^\cdot \lambda} \tilde{\eta}^\tilde{A} \tilde{B}\right) q_A,$$

where we have made use of Eq. (60). We also want the $\lambda$ derivative of $U$

$$U_{,\lambda} = -\left[\eta^{\lambda\tilde{\lambda}} + \frac{r_{,\lambda}^\cdot B}{r_{,\lambda}^\cdot} \tilde{\eta}^\tilde{A} \tilde{B}\right] q_A + 2 \beta_{,\lambda} \left(U + \tilde{\eta}^{\lambda\tilde{A}} q_{,\lambda}\right),$$

where in the last line we have used Eq. (68) to eliminate $r_{,\lambda\lambda}$.

Then, $U$ is found to second-order accuracy by:

$$U(y^\alpha) = U + U_{,\lambda} \lambda + O(\lambda^2).$$

4.6.4. The “mass aspect” $W$

The metric function $V$ is given in terms of $\eta^{rr}$ and $\eta^{ru}$ by

$$V \equiv -\frac{r^{rr}}{\eta^{ru}}.$$

For Minkowski-space, $V = r$ at infinity. Thus, we introduce the auxiliary metric function $W \equiv (V - r)/r^2$, which is regular at null infinity. In terms of the contravariant null metric (with the affine parameter $\lambda$ as the radial coordinate)

$$W = \frac{1}{r} \left(\frac{\eta^{rr}}{r_{,\lambda}^\cdot} - 1\right) = \frac{1}{r} \left(r_{,\lambda}^\cdot \tilde{\eta}^{\lambda\tilde{\lambda}} + 2 \left(r_{,\tilde{A}}^\cdot \tilde{\eta}^{\lambda\tilde{\lambda}} - r_{,u}\right) + \frac{r_{,\tilde{A}}^\cdot r_{,\tilde{B}}}{r_{,\lambda}^\cdot} \tilde{\eta}^{\tilde{A} \tilde{B}} - 1\right),$$

The $\lambda$ derivative of $W$ is given by

$$W_{,\lambda} = -\frac{r_{,\lambda}}{r} W + \frac{1}{r} \left(r_{,\lambda}^\cdot \tilde{\eta}^{\lambda\tilde{\lambda}} + 2 \left(r_{,\tilde{A}}^\cdot \tilde{\eta}^{\lambda\tilde{\lambda}} - r_{,u}\right) + \frac{r_{,\tilde{A}}^\cdot r_{,\tilde{B}}}{r_{,\lambda}^\cdot} \tilde{\eta}^{\tilde{A} \tilde{B}} - 1\right),$$

$$= -\frac{r_{,\lambda}}{r} \left(\frac{r_{,\lambda}}{r} + 2 \beta_{,\lambda}\right) \tilde{\eta}^{\lambda\tilde{\lambda}} - \tilde{\eta}^{\lambda\tilde{\lambda}} - \frac{1}{r} \right) + \frac{2}{r} \left(r_{,\lambda}^\cdot u - r_{,\lambda u}\right)$$

$$+ \frac{2}{r} \left(r_{,\tilde{A}}^\cdot \tilde{\eta}^{\lambda\tilde{\lambda}} + 2 \beta_{,\lambda} r_{,\tilde{A}}^\cdot \tilde{\eta}^{\lambda\tilde{\lambda}} - \frac{r_{,\tilde{A}}^\cdot u}{r} \tilde{\eta}^{\tilde{A} \tilde{B}}\right) - \frac{r_{,\tilde{A}}^\cdot \tilde{B}}{r^2} \tilde{\eta}^{\tilde{A} \tilde{B}}.$$
Then, $W$ is found to second-order accuracy by:
\[ W(y^\alpha) = W + W,\lambda \lambda + O(\lambda^2). \tag{80} \]

5. Injection

We have now reached the halfway point in the problem of relating data between the Null and Cauchy computational approaches. We turn to injection, the final part of the problem. Injection is the inverse problem to extraction, and allows us to use data obtained by characteristic evolution in the exterior of the world-tube in order to provide the exact boundary conditions for Cauchy evolution in its interior. That is, given the metric in Bondi coordinates in a region around the world-tube $\Gamma$, two steps must be carried out. The first ingredient is to relate the Cartesian coordinate system to the Bondi null coordinates. Secondly, the Cartesian metric components must be calculated in the neighborhood of $\Gamma$ in the usual way, from the Bondi metric components and the Jacobian of the coordinate transformation.

5.1. LOCATING THE CARTESIAN GRID WORLDLINES

Given a worldline of a Cartesian grid point, we need to locate, in null coordinates, its intersection with a given null hypersurface. Mathematically, this means: Given $x^i$ and $u$ we want to find $t$ and the null coordinates $r$, as well as $y^A = y^A(x^{(0)i}) = (q, p)$ (where, at this stage, $x^{(0)i}$ is unknown).

The starting point is the geodesic equation Eq. (27)
\[ x^\alpha = x^{(0)\alpha} + \lambda \ell^{(0)\alpha} + O(\lambda^2), \tag{81} \]
Here $\ell^{(0)\alpha} = \ell^\alpha(u, y^A(x^{(0)i}))$ is the value of the null vector given by Eq. (26) at the point on the world-tube with null coordinates $u = t^{(0)}$, $\lambda = 0$ and $y^A(x^{(0)i})$.

We set $L^\alpha \equiv \ell^\alpha(u, y^A(x^i))$, so that
\[ \ell^{(0)\alpha} \equiv \ell^\alpha(x^{(0)\beta}) = L^\alpha + O(\lambda), \tag{82} \]
since $y^A(x^i) = y^A(x^{(0)i}) + O(\lambda)$. ($L^\alpha$ can now be interpolated onto the stereographic coordinate patch to fourth order accuracy in terms of known quantities near the world tube.)

To the same approximation as (81), we have
\[ x^\alpha = x^{(0)\alpha} + \lambda L^\alpha + O(\lambda^2) \tag{83} \]
so that we have four equations for the five unknowns $(x^{(0)i}, t, \lambda)$:
\[ t = u + \lambda L^t + O(\lambda^2) \tag{84} \]
\[ x^i = x^{(0)i} + \lambda L^i + O(\lambda^2). \tag{85} \]
To find the fifth unknown, we need one additional equation introducing new information. This is conveniently supplied by the equation defining the world-tube Eq. (20). Even though we have not yet found the values for \(x^{(0)i}\), we may use Eq. (20) to eliminate these unknowns by taking the Euclidean norm of Eq. (85), whence using Eq. (19) we find:

\[
R^2 = \hat{r}^2 + \lambda^2 (L \cdot L) - 2\lambda (L \cdot x) + O(\lambda^2). \tag{86}
\]

where the value of \(R^2 = (x^{(0)} \cdot x^{(0)})\) is known from the beginning by the definition of the world tube, and \(\hat{r}^2 = (x \cdot x)\).

This is a quadratic in \(\lambda\), but we are consistently only keeping terms to linear order. This leads to

\[
\Lambda = (\hat{r}^2 - R^2)/[2(L \cdot x)] \tag{87}
\]

Consequently, \(\Lambda = \lambda + O(\lambda^2)\) and can be calculated in terms of known quantities. This leaves four unknown quantities remaining. To proceed to evaluate these in terms of known data, we set

\[
T = u + \Lambda L^i, \quad X^{(0)i} = (X^{(0)}, Y^{(0)}, Z^{(0)}) = x^i - \Lambda L^i, \quad \text{and} \quad Y^A = (Q, P) = y^A(X^{(0)i}).
\]

Then, using Eq. (18)

\[
Q = \frac{X^{(0)}}{R \pm Z^{(0)}}, \quad P = \frac{\pm Y^{(0)}}{R \pm Z^{(0)}}, \tag{88}
\]

on the north (+) and south (−) patches. \(T, \Lambda \) and \(Y^A\) are accurate to \(O(\lambda^2)\) since \(t = T + O(\lambda^2), \lambda = \Lambda + O(\lambda^2)\) and \(y^A = Y^A + O(\lambda^2)\).

Finally, the value of \(r\) is obtained from

\[
r = r^{(0)} + r_{\alpha}^{(0)} \Lambda, \tag{89}
\]

and the values of \(r_{,\lambda}, r_{,A}\) and \(r_{,u}\) (used in computing the \(\tilde{\eta}^{\hat{\alpha}\hat{\beta}}\) metric) from

\[
r_{,\lambda} = r_{,\alpha}^{(0)} + r_{,\lambda\lambda}^{(0)} \Lambda, \quad r_{,A} = r_{,A}^{(0)} + r_{,\lambda A}^{(0)} \Lambda, \quad r_{,u} = r_{,u}^{(0)} + r_{,\lambda u}^{(0)} \Lambda \tag{90}
\]

all to \(O(\lambda^2)\) accuracy.

We calculate \(r^{(0)}\), the derivatives \(r_{,\lambda}^{(0)}, r_{,A}^{(0)}\) and \(r_{,u}^{(0)}\) and the mixed derivatives \(r_{,\lambda\lambda}^{(0)}, r_{,\lambda A}^{(0)}\) and \(r_{,\lambda u}^{(0)}\) at the points \((Q, P)\) on the world-tube by fourth order interpolation.

The null metric variables are then obtained by fourth order interpolation at the Bondi coordinate points \((r, Q, P, u)\), corresponding to the Cartesian coordinate points \((x^i, T)\)

5.2. REVERSING THE COORDINATE TRANSFORMATION

The following describes the procedure to obtain the contravariant null metric \(\tilde{\eta}^{\hat{\alpha}\hat{\beta}}\) in affine coordinates \(\tilde{y}^\alpha = (u, q, p, \lambda)\) on points on the characteristic
This is 90% of the work in obtaining the Cartesian metric at those points. What remains is to contract this null metric with the Jacobian of the coordinate transformation $x^\mu = x^\mu(\tilde{y}^\alpha)$. The Jacobian is given in Eq. (32) as a series expansion on the parameter $\lambda$. We will use this expression, and consequently we need to work with the contravariant (rather than the covariant) metric components, since they will transform with the already known Jacobian as:

$$g^{\mu\nu} = \frac{\partial x^\mu}{\partial \tilde{y}^\alpha} \frac{\partial x^\nu}{\partial \tilde{y}^\beta} \tilde{\eta}^{\tilde{\alpha} \tilde{\beta}}. \quad (91)$$

### 5.2.1. The metric on the sphere

Recall that on each stereographic patch we introduce complex null vectors on the sphere $q^A = (P/2)(\delta^A_2 + i\delta^A_3)$ where $P = 1 + \xi \bar{\xi}$ and the $q^A$ satisfy the orthogonality condition $\bar{q}_A q^A = 2$. The $q^A$ define a metric on the sphere $q_{AB} = (4/P^2)\delta_{AB}$ and $q_A = (2/P)(\delta^\alpha_A + i\delta^\beta_A) = q_{AB}q^B$.

By construction, the null metric restricted to the sphere, $\eta_{AB}$, is the same in Bondi coordinates $y^\alpha$ and affine coordinates $\tilde{y}^\tilde{\alpha}$. It can be expanded as:

$$\tilde{\eta}_{\tilde{A}\tilde{B}} \equiv \eta_{AB} = \alpha q_A q_B + \bar{\alpha} \bar{q}_A \bar{q}_B + \delta q_A \bar{q}_B + \bar{\delta} \bar{q}_A q_B \quad (92)$$

The values of $\alpha$ and $\delta$ follow from the orthogonality condition

$$4\alpha = \eta_{AB} q^A q^B, \quad 4\delta = \eta_{AB} \bar{q}^A \bar{q}^B = 4\bar{\delta}, \quad (93)$$

From the definition of $J$ and $K$

$$J = \frac{1}{2} q^A q^B h_{AB}, \quad K = \frac{1}{2} q^A \bar{q}^B h_{AB}, \quad (94)$$

and $\eta_{AB} = r^2 h_{AB}$, it follows that

$$\alpha = \frac{1}{2} r^2 J, \quad \delta = \frac{1}{2} r^2 K, \quad (95)$$

so we can write the metric on the sphere in terms of $J$ and $K$ as

$$\eta_{AB} = \frac{1}{2} r^2 (J q_A q_B + \bar{J} \bar{q}_A \bar{q}_B + K q_A \bar{q}_B + K \bar{q}_A q_B) \quad (96)$$

From the expressions for the $q^A$, the components of the sphere metric are given by:

$$\eta_{qq} = \frac{4r^2}{P^2} (K + R(J)), \quad \eta_{pp} = \frac{4r^2}{P^2} (K - R(J)), \quad \eta_{qp} = \frac{4r^2}{P^2} \Im(J) \quad (97)$$
Notice that given the Bondi coordinates of a point, the determinant is known
\[ \det(\eta_{AB}) = r^4 \det(q_{AB}) = 16 r^4 / P^4, \]
(98)
therefore the inverse sphere metric \( \eta^{AB} \) such that \( \eta^{AB} \eta_{BC} = \delta^A_C \) has coefficients
\[
\eta^{qq} = \tilde{\eta}^{\tilde{q}\tilde{q}} = \frac{P^2}{4 r^2} (K - \Re(J)),
\eta^{pp} = \tilde{\eta}^{\tilde{p}\tilde{p}} = \frac{P^2}{4 r^2} (K + \Re(J)),
\eta^{qp} = \tilde{\eta}^{\tilde{q}\tilde{p}} = -\frac{P^2}{4 r^2} \Im(J).
\]
(99)

5.2.2. The radial-angular metric coefficients
We can write the metric coefficients in terms of a single coefficient \( \gamma \)
\[
\tilde{\eta}^{\lambda\tilde{A}} = \gamma q^{\lambda} + \gamma \bar{q}^{\tilde{A}}
\]
(100)
In components
\[
\tilde{\eta}^{\lambda p} = P \Re(\gamma), \quad \tilde{\eta}^{\lambda q} = P \Im(\gamma)
\]
(101)
The value of \( \gamma \) follows from the expression for the metric function \( U \)
\[
U = U^A q_A = \frac{\eta^A}{\eta^{uu}} q_A = -\left( \eta^{\lambda\tilde{A}} + \frac{r,\beta}{r,\lambda} \tilde{\eta}^{\tilde{A}\tilde{B}} q_{\tilde{A}} \right) q_{\tilde{A}},
\]
(102)
\[
2 \gamma = -U - \frac{r,\beta}{r,\lambda} \tilde{\eta}^{\tilde{A}\tilde{B}} q_{\tilde{A}}
\]
(103)
Recall that the derivatives \( r,\lambda, r,u \) are at constant \( \lambda \) and \( r,\lambda \) can be read off directly from the Bondi metric function \( \beta \)
\[
r,\lambda = e^{-2\beta}
\]
(104)
From the expressions for \( \tilde{\eta}^{\tilde{A}\tilde{B}} \) and \( q_{\tilde{A}} \),
\[
r,\beta \tilde{\eta}^{\tilde{A}\tilde{B}} q_{\tilde{A}} = \frac{2}{P} [r,2 (\tilde{\eta}^{pp} + i \tilde{\eta}^{pq}) + r,3 (\tilde{\eta}^{pq} + i \tilde{\eta}^{qq})]
= \frac{P}{2 r^2} [r,2 (K - J) + ir,3 (K + J)]
\]
(105)
thus the complex coefficient sought is given by
\[
\gamma = -\frac{1}{2} U - e^{2\beta} \frac{P}{4 r^2} [r,2 (K - J) + ir,3 (K + J)]
\]
(106)
The $r_A$ can be obtained at the point where the coordinate transformation is being performed to $O(\lambda^2)$, by using the angular derivatives of $r_\lambda$. To this end, note that for fixed $(q,p)$:

$$r_A = r_A^{(0)} + r_A \lambda \lambda$$  \hspace{1cm} (107)

where the derivatives on the right hand side are computed on the world-tube.

5.2.3. The $\tilde{\eta}^\lambda\lambda$ metric function

By reversing the procedure to obtain $W$, i.e. from

$$W = \frac{1}{r} \left( r_\lambda \tilde{\eta}^{\lambda\lambda} + 2 \left( r_{,A} \tilde{\eta}^{\lambda\tilde{A}} - r_{,u} \right) + \frac{r_{,A} r_{,B} \tilde{\eta}^{\tilde{A}\tilde{B}}}{r_\lambda} - 1 \right)$$  \hspace{1cm} (108)

we obtain the remaining component of the null metric

$$\tilde{\eta}^{\lambda\lambda} = e^{2\beta} \left( rW + 1 - 2 \left( r_{,A} \tilde{\eta}^{\lambda\tilde{A}} - r_{,u} \right) - e^{2\beta} r_{,A} r_{,B} \tilde{\eta}^{\tilde{A}\tilde{B}} \right)$$  \hspace{1cm} (109)

We have made use of the relation $r_\lambda = e^{-2\beta}$. The $r_{,u}$ and $r_{,\tilde{A}}$ are at constant $\lambda$, the former can be evaluated to $O(\lambda)$ accuracy by using the value at the world-tube. To get $r_{,u}$ to $O(\lambda^2)$, we need to calculate $r_{,\lambda u} = -2 e^{-2\beta} \beta_{,u}$ on the world-tube, and use $r_{,u} = r_{,u}^{(0)} + r_{,\lambda u} \lambda$.

This completes the calculation of the final contravariant metric component, and so the injection process may be carried out at last, after the final multiplication by the Jacobian described in Eq. (91).

5.2.4. Status of the algorithm

The CCM algorithm described in the previous sections is quite new. It has not yet been translated into a stable numerical scheme for black hole collisions and interactions in 3-D. However, there has already been extensive testing of these techniques in simpler situations. Recently, significant codes have been built which implement these ideas for scalar waves without gravity but with full 3-D Cartesian and null spherical coordinate grid patches in flat space [17, 18]. Codes have also been written for 1-D problems with gravitation, both for spherical self-gravitating scalar waves collapsing and forming black holes [19, 20] and for cylindrically symmetric vacuum geometry [21, 22]. What has not yet been accomplished is the development of stable codes with both 3-D geometry and non-trivial strong gravitation, although codes currently under development demonstrate the stable evolution of a single moving black hole. Thus, we may expect exciting progress...
in the near future, and the mysterious details of collision between black holes may soon be unveiled.

5.3. ACKNOWLEDGEMENTS

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