TOPICAL REVIEW

Boundary conditions for the gravitational field

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Abstract

A review of the treatment of boundaries in general relativity is presented with the emphasis on application to the formulations of Einstein’s equations used in numerical relativity. At present, it is known how to treat boundaries in the harmonic formulation of Einstein’s equations and a tetrad formulation of the Einstein–Bianchi system. However, a universal approach valid for other formulations is not in hand. In particular, there is no satisfactory boundary theory for the 3+1 formulations which have been highly successful in binary black hole simulation. I discuss the underlying problems that make the initial-boundary-value problem much more complicated than the Cauchy problem. I review the progress that has been made and the important open questions that remain.

*Science is a differential equation. Religion is a boundary condition.*
(Alan Turing, quoted in J D Barrow, ‘Theories of Everything’)

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1. Introduction

There are no natural boundaries for the gravitational field analogous to the conducting boundaries that play a major role in electromagnetism. In principle, there is no need to introduce any. The behavior of the universe as a whole can be posed as an initial-value (Cauchy) problem. In an initial-value problem, data are given on a spacelike hypersurface $S_0$. The problem is to determine a solution in the future domain of dependence $D^+(S_0)$, which consists of those points whose past-directed characteristics all intersect $S_0$. The problem is well-posed if there exists a unique solution which depends continuously on the initial data. The pioneering work of Bruhat [1] showed that the initial-value problem for the (classical) vacuum gravitational field is well-posed. Assuming that matter fields do not spoil things, this suggests that the global cosmological problem of treating the universe as a whole can be solved in a physically meaningful way, i.e. in a way such that the solution does not undergo uncontrolled variation under a perturbation of the initial data. This is indeed the case for the presently accepted cosmological model of an accelerating universe (positive cosmological constant) where the conformal boundary at future null infinity $I^+$ is spacelike. In a conformally compactified picture, $I^+$ acts as a spacelike cap on the future evolution domain and no boundary condition is necessary or indeed allowed.

In practice, of course, treating an isolated system as part of a global cosmological spacetime is too complicated a problem without oversimplifying assumptions such as isotropy or homogeneity. One global approach applicable to isolated systems is to base the Cauchy problem on the analog of a foliation of Minkowski spacetime by the hyperboloidal hypersurfaces

$$t^2 - x^2 - y^2 - z^2 = T^2, \quad t \geq T.$$

(1.1)

In a Penrose conformally compactified picture [2], this foliation asymptotes to the light cones and extends to a foliation of future null infinity $I^+$. The analog in curved spacetime is a foliation by positive constant mean curvature hypersurfaces. Since no light rays can enter an asymptotically flat spacetime through $I^+$, no boundary data are needed to evolve the interior spacetime. In addition, the waveform and polarization of the outgoing radiation can be unambiguously calculated at $I^+$ in terms of the Bondi news function [3]. This approach was first extensively developed by Friedrich [4] who formulated a hyperbolic version of the Einstein–Bianchi system of equations, which is manifestly regular at $I^+$, in terms of the
conformally rescaled metric, connection and Weyl curvature. This is potentially the basis for a very attractive numerical approach to simulate global problems such as gravitational wave production. For reviews of progress on the numerical implementation, see [5–7]. There has been some success in simulating model axisymmetric problems [8]. More recently, there have been other attempts at the hyperboloidal approach based upon the Einstein equations for the conformal metric. Zenginoğlu [9] has implemented a code based upon a generalized harmonic formulation in which the gauge source terms produce a hyperbolic foliation. A mixed hyperbolic–elliptic system proposed by Moncrief and Rinne [10] has been implemented as an axisymmetric code [11] which produces long-term stable evolutions. Another hyperbolic–elliptic system based upon a tetrad approach has been developed by Bardeen, Sarbach and Buchman [12]. In spite of the attractiveness of the hyperboloidal approach and its success with model problems, considerable work remains to make it applicable to systems of astrophysical interest.

A different global approach is to match the Cauchy evolution inside a finite worldtube to an exterior characteristic evolution extending to \( I^+ \). In this approach, called Cauchy-characteristic matching, the characteristic evolution is constructed by using the Cauchy evolution to supply characteristic data on an inner worldtube, while the characteristic evolution supplies the outer boundary data for the Cauchy evolution. The success of Cauchy-characteristic matching depends upon the proper mathematical and computational treatment of the initial-boundary-value problem (IBVP) for the Cauchy evolution. This approach has been successfully implemented in the linearized regime [13] but also needs considerable additional work to apply to astrophysical systems. See [14] for a review.

Instead of a global treatment, the standard approach in numerical relativity, as in computational studies of other hyperbolic systems, is to introduce an artificial outer boundary. Ideally, the outer boundary treatment is designed to represent a passive external universe by allowing radiation to cross only in the outgoing direction. This is the primary application of the IBVP. Other possible applications, which I will not consider, are the timelike conformal boundary to a universe with negative cosmological constant and the membranes which play a role in higher dimensional theories. While there are no natural boundaries in classical gravitational theory, boundaries do play a central role in the ideas of holographic duality introduced in higher dimensional attempts at quantum gravity. Such applications are also beyond the scope of this review as well as beyond my own expertise. Here, I confine my attention to four-dimensional spacetime, although the techniques governing a well-posed IBVP readily extend to hyperbolic systems in any dimension.

In the IBVP, data on a timelike boundary \( T \), which meets \( S_0 \) in a surface \( B_0 \), are used to further extend the solution of the Cauchy problem to the domain of dependence \( D^+ (S_0 \cup T) \). In the simulation of an isolated astrophysical system containing neutron stars and black holes, the outer boundary \( T \) is coincident with the boundary of the computational grid and \( B_0 \) is topologically a sphere surrounding the system. However, for purposes of treating the underlying mathematical and computational problems, it suffices to concentrate on the local problem in the neighborhood of some point on the intersection \( B_0 \) between the Cauchy hypersurface \( S_0 \) and the boundary \( T \). For hyperbolic systems, the global solution in the spacetime manifold \( \mathcal{M} \) can be obtained by patching together local solutions. This is because the finite speed of propagation allows localization of the problem. The setting for this local problem is depicted in figure 1.

The IBVP for Einstein’s equations only received widespread attention after its importance to the artificial outer boundaries used in numerical relativity was pointed out [15]. The first strongly well-posed IBVP was achieved for a tetrad version of the Einstein–Bianchi system, expressed in first differential order form, which included the tetrad, connection and curvature
Figure 1. Data on the 3-manifolds $S_0$ and $T$, which intersect in the 2-surface $B_0$, locally determine a solution in the spacetime manifold $\mathcal{M}$. 

Tensor as evolution fields [16]. Strong well-posedness guarantees the existence of a unique solution which depends continuously on both the Cauchy data and the boundary data. A strongly well-posed IBVP was later established for the harmonic formulation of Einstein’s equations as a system of second-order quasilinear wave equations for the metric [17]. The results were further generalized in [18, 19] to apply to a general quasilinear class of symmetric hyperbolic systems whose boundary conditions have a certain hierarchical form.

A review of the IBVP in general relativity must per force be of a different nature than a review of the Cauchy problem. The local properties of the Cauchy problem are now well understood. Several excellent reviews exist [20–23]. For the IBVP, the results are not comprehensive and are closely tied to the choice of hyperbolic reduction of Einstein’s equations. There are only a few universal features and, in particular, there is no satisfactory treatment of the 3+1 formulation which is extensively used in numerical relativity. For that reason, I will adopt a presentation which differs somewhat from the standard approach with the motivation of setting up a bare bones framework whose flexibility might be helpful in further investigations.

My presentation is also biased by the important role of the IBVP in numerical relativity, which treats Einstein’s equations as a set of partial differential equations (PDEs) governing the metric in some preferred coordinate system. On the other hand, from a geometrical perspective, one of the most fundamental and beautiful results of general relativity is that the properties of the local Cauchy problem can be summed up in geometric terms independent of any coordinates or explicit PDEs. This geometric formulation only came about after the Cauchy problem was well understood from the PDE point of view. The importance of the geometric approach to the numerical relativist is that it supplies a common starting point for discussing and comparing different formulations of Einstein’s equations. Presently, the PDE aspects of metric formulations of the IBVP are only understood in the harmonic formulation. In order to transfer this insight into other formulations, a geometric framework can serve as an important guide. For that reason, I will shift often between the PDE and geometric approach. When the emphasis is on the geometric side, I will use abstract indices, e.g. $v^a$ to denote a vector field,
and on the PDE side, I will use coordinate indices, e.g. \( v^\mu = (v^t, v^i) \), to denote components with respect to the spacetime coordinates \( x^\mu = (t, x^i) \).

The standard mathematical approach to the IBVP is to first establish the well-posedness of the underlying Cauchy problem, and next the local half-space problem. If these individual problems are well-posed (in a sense to be qualified later), then the problems with more general boundaries will also be well-posed. Thus, I start my review in section 2 by first providing some brief background material for the Cauchy problem.

Next, in section 3, I point out the complications in going from the Cauchy problem to the IBVP. The IBVP for Einstein’s equations is not well understood due to problems arising from the constraint equations. The motivation for this work stems from the need for an improved understanding and implementation of boundary conditions in the computational codes being used to simulate binary black holes. The ability to compute the details of the gravitational radiation produced by compact astrophysical sources, such as coalescing black holes, is of major importance to the success of gravitational wave astronomy. If the simulation of such systems is based upon a well-posed Cauchy problem but not a well-posed IBVP, then the results cannot be trusted in the domain of dependence of the outer boundary. In sections 4–6, I present the underlying mathematical theory.

Early computational work in general relativity focused on the Cauchy problem and the IBVP only received considerable attention after its importance to stable and accurate simulations was recognized. I discuss some history of the work on the IBVP in section 7, for the purpose of pointing out some of the partial successes and ideas which may be of future use.

In addition to the mathematical issue of an appropriate boundary condition, the description of a binary black hole as an isolated system raises the physical issue of the appropriate outer boundary data. In the absence of an exterior solution, which could provide these data by matching, the standard practice is to set these data to zero. This raises the question, discussed in section 8, of how to formulate a non-reflecting outer boundary condition in order to avoid spurious incoming radiation.

Sections 9 and 10 describe the two strongly well-posed formulations of the IBVP, which are known at the present time. Neither is based upon a 3 + 1 formulation and both of them handle the constraints in different ways. This prompts the discussion, in section 11, of constraint enforcement in the 3+1 formulations. The resolution of issues regarding geometric uniqueness, discussed in section 12, would shed light on the universal features of the IBVP that would perhaps guide the way to a successful 3 + 1 treatment.

There is also the computational problem of turning a well-posed IBVP into a stable and accurate evolution code. I will not go into the details of the large range of techniques which are necessary for the successful implementation of a numerical relativity code. Since initiating this review, I have learned of a separate review in progress [24] which covers such numerical techniques in great detail. Building a numerical relativity code is a complex undertaking. As observed by Post and Votta [25] in a study of large-scale computational projects, ‘the peer review process in computational science generally doesn’t provide as effective a filter as it does for experiment or theory. Many things that a referee cannot detect could be wrong with a computational science paper...The few existing studies of error levels in scientific computer codes indicate that the defect rate is about seven faults per 1000 lines of Fortran’. They emphasize that ‘New methods of verifying and validating complex codes are mandatory if computational science is to fulfill its promise for science and society’. These observations are especially pertinent for numerical relativity where validation by agreement with experiment is not yet possible. In that spirit, I discuss the code tests that have been proposed and carried out for the gravitational IBVP in section 13.
My aim has been to present the background material which might open new avenues for a better understanding of the IBVP and lead to progress on some of the important open questions posed in section 14.

2. The Cauchy problem

Here I summarize those aspects of the Cauchy problem which are fundamental to the IBVP. For more detail, see [20–23].

In contrast to Newtonian theory, which describes gravity in terms of an elliptic Poisson equation that propagates the gravitational field instantaneously, the retarded interactions implicit in general relativity give rise to new features such as gravitational waves. Wave propagation results from the mathematical property that Einstein’s equations can be reduced to a hyperbolic system of PDEs. However, the coordinate freedom in Einstein’s theory admits gauge waves which propagate with arbitrarily high speeds, including speeds faster than light. Einstein’s equations are not a priori a hyperbolic system in which propagation speeds must be bounded and for which an initial-value problem can be posed.

This crucial step in going from Einstein’s equations to a hyperbolic system has been highlighted by Friedrich as the process of hyperbolic reduction [26]. The first and most famous example of hyperbolic reduction was through the introduction of harmonic coordinates, which led to the classic result that the Cauchy problem for the harmonic formulation of Einstein’s equations is well-posed [1]. Here I summarize the hyperbolic reduction of Einstein’s equations in terms of the generalized harmonic coordinates $x^\alpha = (t, \mathbf{x}) = (t, x, y, z)$, which are functionally independent solutions of the curved-space scalar-wave equation

$$\Box x^\mu = \frac{1}{\sqrt{-g}} \partial_\alpha (\sqrt{-g} g^{\mu \beta} \partial_\beta x^\mu) = -\hat{\Gamma}^\mu,$$  \hspace{1cm} (2.1)

where $\hat{\Gamma}^\mu$ are gauge source functions [26]. In terms of the connection $\Gamma^\mu_{\alpha\beta}$, these harmonic conditions are

$$C^\mu := \Gamma^\mu - \hat{\Gamma}^\mu = 0,$$  \hspace{1cm} (2.2)

where

$$\Gamma^\mu_{\alpha\beta} = g^{\mu \beta} \Gamma^\mu_{\alpha \beta} = -\frac{1}{\sqrt{-g}} \partial_\alpha (\sqrt{-g} g^{\mu \alpha}).$$  \hspace{1cm} (2.3)

The hyperbolic reduction of the Einstein tensor results from setting

$$E^{\mu\nu} := G^{\mu\nu} - \nabla^\mu (C^\nu) + \frac{1}{2} g^{\mu\nu} \nabla^\rho C^\rho = 0,$$  \hspace{1cm} (2.4)

where $C^\nu$ is treated formally as a vector field in constructing the ‘covariant’ derivatives $\nabla^\mu C^\nu$. (In generalized harmonic formulations based upon a background connection, $C^\nu$ is a legitimate vector field. See section 10.)

When the harmonic gauge source functions have the functional dependence $\hat{\Gamma}^\nu(x, g)$, the principal part of (2.4) reduces to the wave operator acting on the densitized metric, i.e.

$$E^{\mu\nu} = \frac{1}{2 \sqrt{-g}} \partial_\alpha (\sqrt{-g} g^{\mu\alpha} \partial_\beta (\sqrt{-g} g^{\nu\beta})) + \text{lower order terms}. \hspace{1cm} (2.5)$$

Thus, the harmonic evolution equations (2.4) are quasilinear wave equations for the components of the densitized metric $\sqrt{-g} g^{\mu\nu}$. The well-posedness of the Cauchy problem for the system (2.4) then follows from known results for systems of quasilinear wave equations. (It is important to bear in mind that such results are local in time since there is no general theory for the global existence of solutions to nonlinear equations.)
In turn, the well-posedness of the Cauchy problem for the harmonic Einstein equations also follows provided that the harmonic conditions \( C^\mu = 0 \) are preserved under the evolution. The proof of constraint preservation results from applying the contracted Bianchi identity \( \nabla^\rho C^\mu + R^\mu_\rho C^\rho = 0 \). This leads to a homogeneous wave equation for \( C^\mu \),

\[
\nabla^\rho \nabla_\rho C^\mu + R^\mu_\rho C^\rho = 0.
\]

(2.6)

If the initial data enforce

\[
C^\mu|_{S_0} = 0
\]

(2.7)

and

\[
\partial_t C^\mu|_{S_0} = 0,
\]

(2.8)

then the unique solution of (2.6) is \( C^\rho = 0 \). It is easy to satisfy (2.7) by algebraically determining the initial values of \( \partial_t g^\mu_\nu \) in terms of the initial values of \( g^\mu_\nu \) and their spatial derivatives. In order to see how to satisfy (2.8), note that the reduced equations (2.4) imply

\[
G^{\mu\nu} n_\nu = n_\nu \nabla^{(\mu} C^{\nu)} - \frac{1}{2} n^\rho \nabla_\rho C^\mu,
\]

(2.9)

where

\[
n_\nu = -\frac{1}{\sqrt{-g}} \partial_\nu t
\]

is the unit timelike normal to the Cauchy hypersurfaces. Thus, if

\[
G^{\mu\nu} n_\nu|_{S_0} = 0,
\]

(2.10)

i.e. if the Hamiltonian and momentum constraints are satisfied by the initial data, and if the reduced equations (2.4) are satisfied, then it follows that

\[
[n_\nu \nabla^{(\mu} C^{\nu)} - \frac{1}{2} n^\rho \nabla_\rho C^\mu]|_{S_0} = 0.
\]

(2.11)

It is easy to check that (2.11) implies that \( \partial_t C^\mu|_{S_0} = 0 \) provided \( C^\mu|_{S_0} = 0 \).

As a result, the traditional Hamiltonian and momentum constraints on the initial data, along with the reduced evolution equations (2.4), imply that the initial conditions (2.7) and (2.8) required for preserving the harmonic conditions are satisfied. Conversely, if the Hamiltonian and momentum constraints are satisfied initially, then (2.9) ensures that they will be preserved under harmonic evolution. Thus, the conditions \( C^\nu = 0 \) can be considered as the constraints of the generalized harmonic formulation.

The formalism also allows constraint adjustments by which (2.4) is modified by

\[
E^{\mu\nu} := G^{\mu\nu} - \nabla^{(\mu} C^{\nu)} + \frac{1}{2} g^{\mu\nu} \nabla_\rho C^\rho + A^\mu_\sigma A^\nu_\sigma = 0,
\]

(2.12)

where the coefficients \( A^\mu_\sigma \) have the dependence \( A^\mu_\sigma (x, g, \partial g) \). Such constraint adjustments have proved to be important in applying constraint damping [27] in the simulation of black holes [28–30] and in suppressing long-wavelength instabilities in a shifted gauge wave test [31] (see section 13). However, they do not change the principal part of the reduced equations and have no effect on well-posedness.

Historically, the first Cauchy codes were based upon the ‘3+1’ or Arnowitt–Deser–Misner (ADM) formulation of the Einstein equations [32]. The ADM formulation introduces a Cauchy foliation of spacetime by a time coordinate \( t \) and expresses the four-dimensional metric as

\[
dx^2 = -\alpha^2 dt^2 + h_{ij}(dx^i + \beta^i dt)(dx^j + \beta^j dt),
\]

(2.13)

where \( h_{ij} \) is the induced 3-metric of the \( t = \) const foliation, \( \alpha \) is the lapse and \( \beta^i \) is the shift, with the unit normal to the foliation given by \( n^\mu = (1, -\beta^i)/\alpha \).
The field equations are written in first differential form in terms of the extrinsic curvature of the Cauchy foliation

\[ k_{ij} = \frac{1}{2} \mathcal{L}_n g_{ij}. \]

This can be accomplished in many ways. In one of the earliest schemes proposed for numerical relativity by York [33], the requirement that the six spatial components of the Ricci tensor vanish, i.e. \( R_{ij} = 0 \), yields a set of evolution equations for the 3-metric and extrinsic curvature,

\[
\begin{align*}
\partial_t g_{ij} - \mathcal{L}_\beta g_{ij} &= -2\alpha k_{ij} \\
\partial_t k_{ij} - \mathcal{L}_\beta k_{ij} &= -D_i D_j \alpha + \alpha \left( R_{ij} + k k_{ij} - 2 k_i^j k_{ij} \right),
\end{align*}
\]

where \( D_i \) is the connection and \( R_{ij} \) is the Ricci tensor associated with \( h_{ij} \). The Hamiltonian and momentum constraints take the form

\[
\begin{align*}
2 G^{\mu\nu} n_{\mu} n_{\nu} &= R - k_{ij} k^{ij} + k^2 = 0 \\
G^\mu n_{\mu} &= D_j \left( k^{ij} - h^{ij} k \right) = 0,
\end{align*}
\]

where \( R = h^{ij} R_{ij} \) and \( k = h^{ij} k_{ij} \).

Codes presently used for the simulation of binary black holes apply the constraints to the initial Cauchy data but do not enforce them during the evolution. The choice of evolution equations may be modified by mixing in combinations of the constraint equations. In addition, the evolution equations must be supplemented by equations governing the lapse and shift. There is a lot of freedom in how all this can be done. The choices affect whether the Cauchy problem is well-posed.

3. Complications of the IBVP

The difficulties underlying the IBVP have recently been discussed in [34–37]. There are several chief complications which do not arise in the Cauchy problem.

1. The first complication stems from a well-known property of the flat-space scalar-wave boundary problem

\[
\left( \partial^2_t - \nabla^2 \right) \phi = 0, \quad x \geq 0, \quad t \geq 0.
\]

The light rays are the characteristics of the equation. There are two characteristics associated with each direction, e.g. the characteristics in the \( \pm x \) direction. Both of these characteristics cross the initial hypersurface \( t = 0 \) but only one crosses the boundary at \( x = 0 \). As a result, although the initial Cauchy data consist of the two pieces of information \( \phi|_{t=0} \) and \( \partial_t \phi|_{t=0} \), only half as much boundary data can be freely prescribed at \( x = 0 \), e.g. the Dirichlet data \( q_D = \partial_t \phi|_{t=0} \), or the Neumann data \( q_N = \partial_x \phi|_{t=0} \) or the Sommerfeld data \( q_S = (\partial_t - \partial_x) \phi|_{x=0} \). Sommerfeld data are based upon the derivative of \( \Phi \) in the characteristic direction determined by the outward normal to the boundary. (In the first differential order formalism, \( (\partial_t - \partial_x) \Phi \) is an ingoing variable at the boundary.) The choices \( q_D = q_N = q_S \) do not lead to the same solution. In order to obtain a given physical solution, this implies that the boundary data cannot be prescribed before the boundary condition is specified, i.e. the boundary data for the solution depend upon the boundary condition, unlike the situation for the Cauchy problem. The analog in the gravitational case is the inability to prescribe both the metric and its normal derivative on a timelike boundary, which implies the inability to freely prescribe both the intrinsic 3-metric of the boundary and its extrinsic curvature. This leads to a further complication regarding
constraint enforcement at the boundary, i.e. the Hamiltonian and momentum constraints (2.16) and (2.17) cannot be enforced directly because they couple the metric and its normal derivative.

For computational purposes, a Sommerfeld boundary condition is preferable because it allows numerical noise to propagate across the boundary. Thus, discretization error can leave the numerical grid, whereas Dirichlet and Neumann boundary conditions would reflect the error and trap it in the grid. The Sommerfeld condition on a metric component supplies the value of the derivative \( K^\alpha \partial_\alpha g^{\mu
u} \) in an outgoing null direction \( K^\alpha \). However, the boundary does not pick out a unique outgoing null direction at a given point but, instead, essentially a half-cone of null directions. This complicates the geometric formulation of a Sommerfeld boundary condition. In addition, constraint preservation does not allow free specification of Sommerfeld data for all components of the metric, as will be seen later in formulating the Sommerfeld conditions (10.21)–(10.23).

The correct boundary data for the gravitational field are generally not known except in special cases, e.g. when simulating an exact solution. This differs from electromagnetic theory where, say, homogeneous Dirichlet or Neumann data for the various components of the electromagnetic field correctly describe the data for reflection from a mirror. The tacit assumption in the simulation of an isolated system is that homogeneous Sommerfeld data give rise to minimal back reflection of gravitational waves from the outer boundary. But this is an approximation which only becomes exact in the limit of an infinite-sized boundary.

Another major complication arises from the gauge freedom. In the evolution of the Cauchy data, it is necessary to introduce a foliation of the spacetime by the Cauchy hypersurfaces \( S_t \), with unit timelike normal \( n_a \). The evolution of the spacetime metric

\[
g_{ab} = -n_a n_b + h_{ab}
\]  

is carried out along the flow of an evolution vector field \( t^a \) which is related to the normal by the lapse \( \alpha \) and shift \( \beta^a \) by

\[
t^a = \alpha n^a + \beta^a, \quad \beta^a n_a = 0.
\]  

The choice of foliation is part of the gauge freedom in the resulting solution but does not enter into the specification of the initial data. In the current treatments of the IBVP, the foliation is coupled with the formulation of the boundary condition. As a result, some gauge information enters into the boundary condition and boundary data.

The partial derivative \( \partial_\alpha g^{\mu\nu} \) entering into the construction of the boundary condition for the metric has by itself no intrinsic geometric interpretation, unless, say, a background connection or a preferred vector field is introduced.

In general, the boundary moves with respect to the initial Cauchy hypersurface in the sense that the spacelike unit outer normal \( N_a \) to \( T \) is not orthogonal to the timelike unit normal \( n_a \) to \( S_0 \). The initial velocity of the boundary is characterized by the hyperbolic angle \( \Theta \), where

\[
N^a n_a = \sinh \Theta.
\]  

Specification of \( \Theta \) on the edge \( B_0 \) must be included in the data.

The coordinate specification of the location of the boundary is pure gauge since it does not determine its location geometrically in the sense that a curve is determined geometrically by its acceleration, given its initial position and velocity. Given \( B_0 \) and \( \Theta \), the future location of the boundary should be determined in a geometrically unique way. In the Friedrich–Nagy system, the motion of the boundary is determined by specifying
its mean extrinsic curvature. But this is tantamount to a piece of Neumann data. Can this be accomplished via a non-reflecting boundary condition of the Sommerfeld type?

(7) In a reduction to first differential order form by introducing a momentum $\Pi$, according to the example

$$n^a \partial_a \Phi = \Pi, \quad (3.5)$$

there is a further difficulty if $\Theta \neq 0$ at the boundary. The sign of $\Theta$ determines whether $n^a$ points outward or inward to $\mathcal{T}$, i.e., whether $\Phi$ is an ingoing or outgoing variable.

Thus, the sign of $\Theta$ determines whether such an advection equation requires a boundary condition. This forces a Dirichlet condition on the normal component of the shift in some 3+1 formulations.

(8) There are also compatibility conditions between the initial data and the boundary data at the edge $\mathcal{B}_0$. For the example of the scalar-wave problem (3.1) with a Dirichlet boundary condition at $x = 0$, the boundary data must satisfy

$$\partial_t^2 \Phi|_{(t=0,x=0)} = \left( \partial_t^2 + \partial_x^2 + \partial_y^2 + \partial_z^2 \right) \Phi|_{(t=0,x=0)}, \quad (3.6)$$

where the right-hand side is determined by the initial data. An infinite sequence of such conditions follows from taking time derivatives of the wave equation. They must be satisfied if the solution is required to be $C^\infty$. In simple problems, this sequence of compatibility conditions can be satisfied by choosing initial data and boundary data with support that vanishes in a neighborhood of the edge $\mathcal{B}_0$. But in problems with elliptical constraints, such as those occurring in general relativity, this simple approach is not possible. In numerical relativity, these compatibility conditions are usually ignored, with the consequence that some transient junk radiation emanating from the edge is generated.

In principle, this could be avoided by smoothly gluing the initial data to an exterior region with Schwarzschild [38] or Kerr [39] data. This gluing construction would avoid mathematical difficulties but it is an implicit construction and in practice no numerical algorithm for carrying it out has been proposed. In the simulation of binary black holes, this edge effect combines with another source of junk radiation which is hidden in the choice of initial data. The tacit assumption is that the spurious radiation from these sources is quickly flushed out of the simulation, with no significant effect after a few crossing times. Since this issue is difficult to treat or quantify in a useful way, I adopt the expedient assumption that all compatibility conditions for a $C^\infty$ solution have been met.

In order to resolve most of the above complications, it appears that a foliation $\mathcal{B}_t$ of the boundary $\mathcal{T}$ must be specified as part of the boundary data. Such a foliation is a common ingredient of all successful treatments to date. The foliation supplies the gauge information which determines a unique outgoing null direction for a Sommerfeld condition. In section 4, I specify $\mathcal{B}_t$ in terms of the choice of an evolution vector field on the boundary.

Most of the above complications stem from the fact the domain of dependence determined by the boundary alone is empty. An initial-value problem for a hyperbolic system can be consistently posed in the absence of a boundary. But the opposite is not true for an IBVP. Without an underlying Cauchy problem, an IBVP does not make sense. In an IBVP, boundary data cannot determine a unique solution independently of the initial Cauchy data and there is no domain in which the solution is independent of the initial data. Thus, a well-posed IBVP problem must be based upon a well-posed Cauchy problem.

4. The bare manifold

In constructing an evolution code for the gravitational field, the first step is to define a spatial grid and a time update scheme. This sets up the underlying structure necessary to store the
values of the various fields. The analogous object at the continuum level corresponds to the bare manifold on which the gravitational field is later painted. This is the approach I will adopt here. It provides a useful way to order the introduction of the basic geometric quantities which enter the IBVP.

Setting up the spatial grid corresponds to the analytic specification of the spatial coordinates $x^i$ on $S_0$. The time update algorithm corresponds to the introduction of an evolution field $t^a$ in $\mathcal{M}$ which is tangent to the boundary $\mathcal{T}$. (In more complicated update schemes, which I will not consider, the boundary might move through the grid.) The evolution field must have the property that under its flow, $S_0$ is mapped onto a foliation $S_t$ of $\mathcal{M}$, and its edge $B_0$ is mapped onto a foliation $B_t$ of $\mathcal{T}$.

If a time coordinate is initiated at $t = 0$ on $S_0$, then the flow of $t^a$ induces the adapted coordinates $x^\mu = (t, x^i)$ on $\mathcal{M}$ by requiring

$$\mathcal{L}_t t = 1$$

$$\mathcal{L}_t x^i = 0,$$

where $\mathcal{L}_t$ is the Lie derivative with respect to $t^a$. Note that $t^a$ and the adapted coordinates $x^a$ are explicitly constructed fields on $\mathcal{M}$ with no metric properties. They uniquely fix the gauge freedom on $\mathcal{M}$ in precisely the same way as the numerical grid and update scheme provide a unique evolution algorithm. If $x^A$ are the coordinates on the edge $B_0$, then the corresponding adapted coordinates on the boundary are $(t, x^A)$, where $\mathcal{L}_t x^A = 0$. It will be convenient throughout this review to let the manifold with boundary be described by the adapted coordinates

$$x^\mu = (t \geq 0, x \geq 0, x^A).$$

Under a diffeomorphism $\psi$ of $\mathcal{M}$ which maps $\mathcal{T}$ onto itself, $t^a \rightarrow \psi^* t^a$ where $\psi^* t^a$ can be chosen to be any other possible evolution field. In particular, if $\psi^* t^a = t^a$ in $\mathcal{M}$ and $\psi x^i = x^i$ on $S_0$, then the diffeomorphism must be the identity. Thus, given a coordinate gauge on $S_0$, the choice of $t^a$ determines the remaining diffeomorphism freedom. This allows a description of the evolution in a specific choice of adapted coordinates without losing sight of the gauge freedom.

Note that any 1-form normal to the boundary is proportional to $\partial_t$. However, at the bare manifold level, the unit normal cannot be specified since that involves metric information. The projection tensor

$$\pi^a_b = \delta^a_b - t^a \partial_b t$$

has the properties

$$\pi^a_b v^b \partial_d t = 0,$$

i.e. it projects a vector field into the tangent space of $S_t$, and

$$\pi^a_b u^d u^b = 0,$$

i.e. it projects a 1-form into the space orthogonal to $\partial_t$.

These are the main structures that exist in the IBVP a priori to introducing a geometry on $\mathcal{M}$. There is an alternative approach in which geometrical concepts are introduced earlier. In the Cauchy problem, the initial data can be specified in geometrical form as the tensor fields $\tilde{h}_{ab}$ and $\tilde{k}_{ab}$ on a ‘disembodied’ 3-manifold $\tilde{S}_0$ (cf [40]). Only after the embedding of $\tilde{S}_0$ in $\mathcal{M}$ are these data interpreted as the intrinsic metric $h_{ab}$ and extrinsic curvature $k_{ab}$ of $S_0$. The mean curvature $k = h^{ab}k_{ab}$ can itself be interpreted as a variable determining the location of $S_0$. Similarly, in the IBVP, the mean extrinsic curvature of $\mathcal{T}$ can be interpreted
as a wave equation determining the geometric location of the boundary [16]. However, these interpretations assume knowledge of the spacetime geometry which is only known after a solution is found.

This order in which the basic objects are introduced is akin to the following question: Which came first—the geometry or the manifold (or some combination)? Here I adopt the manifold approach, which is more akin to the spirit of numerical relativity. I assume \textit{a priori}, for the given choice of evolution field $t^a$, that $\mathcal{M}$ is the domain of dependence of the initial-boundary data, i.e. it is the manifold upon which the data determine a unique evolution. Here \textit{‘a priori’} is used in the sense of a spacetime geometry which exists only after the solution of the IBVP is obtained.

5. Initial data

Since Einstein’s equations are second differential order in the metric, any evolution scheme must specify $g_{\mu\nu}$ and $\partial_t g_{\mu\nu}$ on $S_0$. The classic result of the Cauchy problem is that a geometrically unique solution of the Cauchy problem is determined by initial data consisting of the intrinsic metric $h_{ab}$ of $S_0$ and its extrinsic curvature $k_{ab}$, subject to constraints (2.16) and (2.17).

The remaining initial data necessary to specify a unique spacetime metric consist of gauge information, i.e. gauge data that affect the resulting solution only by a diffeomorphism. One such quantity is the lapse $\alpha$, which relates the unit future-directed normal to the time foliation according to

\[ n_a = -\alpha \partial_0. \]  

The embedding of $S_0$ in $\mathcal{M}$ then gives rise to the spacetime metric

\[ g_{ab} = -n_a n_b + h_{ab} \]

and the interpretation of $k_{ab}$ as the extrinsic curvature through the identification

\[ k_{ab} = h^c_a \nabla_c n_b, \]

where $\nabla_c$ is the covariant derivative associated with $g_{ab}$.

The choice of evolution field $t^a$ supplies the remaining gauge data. It is transverse but not in general normal to the Cauchy hypersurface so that it determines a shift $\beta_a$ according to

\[ \beta_a = h_{ab} t^b. \]

This relationship supplies the metric information

\[ g_{ab} t^b = \alpha n_a + \beta_a \]

relating $t^a$ to the unit normal $n_a$.

In the adapted coordinates, the metric has the components

\[ g_{tt} = -\alpha^2 + h_{ij} \beta^i \beta^j \]

\[ g_{ti} = \beta_i = h_{ij} \beta^j \]

\[ g_{ij} = h_{ij}. \]

The inverse metric is given by $g^{ab} = -n^a n^b + h^{ab}$, where

\[ h^{ab} n_b = 0, \quad h^{ae} h_{eb} = \delta^a_b + n^a n_b. \]

In the adapted coordinates,

\[ g^{tt} = -\alpha^{-2} \]
\[ g^{ij} = \alpha^{-2} \mathcal{B}^{ij} \]  
(5.10)

\[ g^{ij} = h^{ij}, \quad h^{ik} h^{kj} = \delta^{ij}. \]  
(5.11)

The implementation of the initial data into an evolution scheme depends upon the details by which Einstein’s equations are converted into a set of PDEs governing \( g_{\mu\nu} \) in the adapted coordinates. All such schemes require specification of the initial values of the lapse and shift, in addition to \( h_{ij} \) and \( k_{ij} \). Thus, it can be assumed that \( g_{ab} \) is specified on \( S_0 \). By Lie transport along the streamlines of \( t^a \), this then allows the construction of a preferred stationary background metric \( \tilde{g}_{ab} \) on \( M \) picked out by the initial data. Given the choice of evolution field \( t^a \) and the initial Cauchy data, this background metric is uniquely and geometrically determined by

\[ L_t \tilde{g}_{ab} = 0, \quad \tilde{g}_{ab} |_{S_0} = g_{ab} |_{S_0}. \]  
(5.12)

In the adapted coordinates, \( \tilde{g}_{\mu\nu}(t, x^i) = g_{\mu\nu}(0, x^i) \).

6. Hyperbolic IBVPs

There is an extensive mathematical literature on the IBVP for hyperbolic systems. The major progress traces back to the formulation of maximally dissipative boundary conditions for linear symmetric hyperbolic systems due to Friedrichs [41] and Lax and Phillips [42]. There has been recent progress in obtaining results for quasilinear systems where the boundary contains characteristics, as arises in some formulations of Einstein’s equations. Unfortunately, much of this material is heavy on the mathematical side and not easy reading for relativists coming from astrophysical or numerical backgrounds. In the absence of the complications of shocks introduced by hydrodynamic sources, relativists are content to deal with smooth, i.e. \( C^\infty \), solutions and forgo the Sobolev theory which enters a complete discussion of the quasilinear IBVP. For relativists, the most readable source on the theory of hyperbolic boundary problems is the textbook by Kreiss and Lorenz [43], which boasts the following: ‘In parts, our approach to the subject is low-tech.... Functional analytical prerequisites are kept to a minimum. What we need in terms of Sobolev inequalities is developed in an appendix.’ Taylor’s [44, 45] treatises on PDEs contain a classic treatment of pseudo-differential theory but are less readable for relativists. Fortunately, much of the critical formalism pertinent to Einstein’s equations appears as background material in papers on the gravitational IBVP. The material I present here is heavily based upon those sources, namely [16, 15, 37, 43, 17–19].

There are two distinct formulations of the IBVP, depending upon whether you consider Einstein’s equations as a natural second differential order system of wave equations or whether you reduce it to a first-order system. While the second-order approach is the most economical, it is not applicable to all formulations of Einstein’s equations, particularly those whose gauge conditions do not have the semblance of wave equations. The first-order theory has been extensively developed because of its historic importance to the symmetric hyperbolic formulation of hydrodynamics. The IBVP for second-order systems has received less attention and some new techniques have originated in the consideration of the Einstein problem.

There are also two distinct approaches to studying well-posedness—one based upon energy estimates and the other based upon pseudo-differential theory where Fourier–Laplace expansions are used to reduce the differential operators to algebraic operators. The pseudo-differential theory can be applied equally well to first- or second-order systems. In the following, I give a brief account of the underlying ideas in terms of some simple model problems. This will provide a background for discussing the difficulties that arise when considering constraint preservation in the gravitational IBVP.
The subclasses of hyperbolic systems consist of weak hyperbolicity, strong hyperbolicity, symmetric hyperbolicity and strict hyperbolicity. These subclasses are determined by the principal part of the system when written as first differential order PDEs. Weakly hyperbolic systems do not have a well-posed Cauchy problem, which turned out to be responsible for the instabilities encountered in early attempts at numerical relativity using naive ADM formulations with a prescribed lapse and shift. Strong hyperbolicity is sufficient to guarantee a well-posed Cauchy problem but not a well-posed IBVP. It is possible to base a well-posed IBVP on either symmetric hyperbolic or strictly hyperbolic systems. However, strictly hyperbolic systems arise very rarely and, to my knowledge, not at all in numerical relativity. So I will limit my discussion to the symmetric hyperbolic case.

I begin with the IBVP for a second-order scalar-wave equation, where the underlying techniques are transparent rather than hidden in the machinery of symmetric hyperbolic theory. The generalization to systems of quasilinear wave equations, described in section 6.1.3, can also be treated by the same techniques as for symmetric hyperbolic systems. However, for application to the harmonic Einstein problem, the scalar treatment suffices since the principal part of the system consists of a common wave operator acting on the individual components of the metric. The mathematical analysis which is necessary for a treatment of the quasilinear IBVP in full rigor is beyond my competence and presumably outside the interest of someone from a more physical or computational background. I simply state the main results and give references when such mathematical theory must be evoked.

6.1. Second-order wave equations

The ideas underlying the well-posedness of the IBVP are well illustrated by the case of the quasilinear wave equation. I give some examples which are relevant to the harmonic formulation of Einstein’s equations and which illustrate the techniques behind both the energy approach and the pseudo-differential approach.

6.1.1. The energy method for second-order wave equations. First, consider the linear wave equation for a scalar field,

$$\Phi_{tt} = \Phi_{xx} + \Phi_{yy} + \Phi_{zz} + F,$$

on the half-space

$$x \geq 0, \quad -\infty < y < \infty, \quad -\infty < z < \infty,$$

with boundary condition at $x = 0$,

$$\Phi_t - \alpha \Phi_x - \beta_2 \Phi_y - \beta_3 \Phi_z = q, \quad \alpha > 0, \beta_2 + \beta_3 < 1,$$

with boundary data $q$, initial data of compact support

$$\Phi = f_1, \quad \Phi_t = f_2, \quad t = 0$$

and forcing term $F(t, x, y, z)$. The subscripts $(t, x, y, z)$ denote partial derivatives, e.g

$$\Phi_t = \frac{\partial \Phi}{\partial t} = \partial_t \Phi.$$

All coefficients and data are assumed to be real and $\alpha > 0, \beta_2, \beta_3$ are constants. The notation

$$(\Phi, \Psi), \quad \|\Phi\|^2 = (\Phi, \Phi) ; \quad (\Phi, \Psi)_B, \quad \|\Phi\|^2_B = (\Phi, \Phi)_B$$

is used to denote the $L_2$ scalar product and norm over the half-space and boundary space, respectively.
In order to adapt the standard definition of energy estimates to second-order systems, the notation \( \Phi = (\Phi_1, \Phi_2, \Phi_3, \Phi_4) \) is used to represent the solution and its derivatives, and similarly \( f = (f_1, f_2, f_3, f_4, f_5) \) for the initial data.

For the scalar IBVP (6.1)–(6.4), strong well-posedness requires the existence of a unique solution satisfying the \textit{a priori} estimate

\[
\|\Phi(t)\|^2 + \int_0^t \|\Phi(\tau)\|^2 d\tau \leq K_T \left( \|f\|^2 + \int_0^t \|F(\tau)\|^2 d\tau + \int_0^t \|q(\tau)\|^2 d\tau \right),
\]

in any time interval \( 0 < t < T \), where the constant \( K_T \) is independent of \( F, f \) and \( q \).

It is important to note that (6.5) estimates the derivatives of \( \Phi \), both in the interior and on the boundary, in terms of the data and the forcing. This is referred to as ‘gaining a derivative’. This property is crucial in extending the local IBVP to global situations, e.g. where the boundary is a sphere or where there is an interior and exterior boundary as in a strip problem. Otherwise reflection from the boundary could lead to the ‘loss of a derivative’, which would lead to unstable behavior under multiple reflections.

The usual procedure is to derive an energy estimate by integration by parts, using for example, \((\Phi_1, \Phi_2) = - (\Phi_2, \Phi_4) = 0\). Consider first the estimates of the derivatives of \( \Phi \) in the homogeneous case \( F = q = 0 \). Using the standard energy for a scalar field, integration by parts gives

\[
\partial_t (\|\Phi_1\|^2 + \|\Phi_2\|^2 + \|\Phi_3\|^2 + \|\Phi_4\|^2) = -2(\partial_t \Phi_1, \Phi_4)_B.
\]

If \( \beta_2 = \beta_3 = 0 \) and \( \alpha > 0 \) in the boundary condition (6.3), then \((\Phi_1, \Phi_3)_B \geq 0\), i.e. the boundary condition is dissipative, and there is an energy estimate. Otherwise there is no obvious way to estimate the boundary flux. Instead, it is possible to use a non-standard energy \( E \) for the scalar-wave equation (6.1) which does provide the key estimate if \( \beta_2^2 + \beta_3^2 > 0 \).

The first step is to show that

\[
E := \|\Phi_1\|^2 + \|\Phi_2\|^2 + \|\Phi_3\|^2 + \|\Phi_4\|^2 - 2(\Phi_1, \beta_2 \Phi_2 + \beta_3 \Phi_3)_B
\]

is a norm for the derivatives \((\Phi_1, \Phi_3, \Phi_2, \Phi_4)\). Since \( \beta_2^2 + \beta_3^2 < 1 \), this follows, after a rotation, from the inequality \( \Phi_1^2 + \Psi^2 - 2\beta \Phi_1 \Psi \geq 0 \) for \( \beta^2 < 1 \).

This leads to

**Lemma 1** The solution of (6.1)–(6.4) satisfies the energy estimate

\[
\partial_t E + \alpha \|\Phi_1\|_B^2 \leq E + \|F\|^2 + \frac{1}{\alpha} \|q\|_B^2.
\]

**Proof.** Integration by parts gives

\[
\partial_t \|\Phi_1\|^2 = 2(\partial_t \Phi_1, \Phi_2)_B = \partial_t (\|\Phi_1\|^2 + \|\Phi_2\|^2 + \|\Phi_3\|^2) + 2(\Phi_1, F) - 2(\Phi_1, \Phi_3)_B
\]

and

\[
2\partial_t (\Phi_1, \beta_2 \Phi_2 + \beta_3 \Phi_3) = 2(\partial_t \Phi_1, \beta_2 \Phi_2 + \beta_3 \Phi_3)_B = -2(\Phi_1, \beta_2 \Phi_2 + \beta_3 \Phi_3)_B + \Phi_1 F, \beta_2 \Phi_2 + \beta_3 \Phi_3)_B
\]

Since (6.3) implies

\[
2(\Phi_1, \Phi_3)_B = 2\alpha \|\Phi_3\|_B^2 + 2(\Phi_1, \beta_2 \Phi_2 + \beta_3 \Phi_3)_B + 2(\Phi_1, q)_B
\]

and subtraction of (6.9) from (6.8) leads to

\[
\partial_t E = 2(\Phi_1 - \beta_2 \Phi_2 - \beta_3 \Phi_3, F) - 2\alpha \|\Phi_3\|_B^2 - 2(\Phi_1, q)_B
\]

\[
\leq \|\Phi_1 - \beta_2 \Phi_2 - \beta_3 \Phi_3\|^2 + \|F\|^2 - \alpha \|\Phi_3\|_B^2 + \frac{1}{\alpha} \|q\|_B^2.
\]
The identity
\[ \| \Phi_t - \beta_2 \Phi_x - \beta_3 \Phi_z \|^2 = E - \| \Phi_x \|^2 - \| \Phi_z \|^2 - \| \Phi_t \|^2 + \| \beta_2 \Phi_x + \beta_3 \Phi_z \|^2 \]
then implies (6.7) and proves the lemma.

By integration, the lemma estimates
\[ E(T) + \int_0^T \| \Phi_t \|_B^2 \, dt \]
\text{in terms of } \ E(0), \ \int_0^T \| F \|^2 \, dt \text{ and } \int_0^T \| q \|^2 \, dt.

Strong well-posedness (6.5) also requires estimates of the boundary norms \( \| \Phi_t \|_B, \| \Phi_x \|_B \) and \( \| \Phi_z \|_B \). First, a calculation similar to that above gives
\[
\partial_t (\Phi_x, \Phi_t) = (\Phi_{xx}, \Phi_{tt}) + (\Phi_x, \Phi_{tt}) + (\Phi_x, \Phi_{yy}) + (\Phi_x, \Phi_{zz}) + (\Phi_t, F)
\]
\[ = -\frac{1}{2} \| \Phi_x \|_B^2 + \frac{1}{2} \| \Phi_z \|_B^2 + \frac{1}{2} \| \Phi_t \|_B^2 + \frac{1}{2} \| \Phi_z \|_B^2 + (\Phi_x, F). \]

\begin{equation}
(6.10)
\end{equation}

Estimates of \( \| \Phi_t \|_B \) in terms of \( \| \Phi_t \|_B, \| \Phi_x \|_B, \| \Phi_z \|_B \) and \( \| q \|_B \) can be obtained from the boundary conditions (6.3), which give, for any \( \delta \) with \( 0 < \delta < 1 \),
\[
\| \Phi_t \|_B^2 = \| \beta_2 \Phi_x + \beta_3 \Phi_z + \alpha \Phi_x + q \|_B^2 \\
\leq \| \beta_2 \Phi_x + \beta_3 \Phi_z \|_B^2 + 2 \| \beta_2 \Phi_x + \beta_3 \Phi_z \|_B \| \alpha \Phi_x + q \|_B + \| \alpha \Phi_x + q \|_B^2 \\
\leq (1 + \delta) \| \beta_2 \Phi_x + \beta_3 \Phi_z \|_B^2 + \left( 1 + \frac{1}{\delta} \right) \| \alpha \Phi_x + q \|_B^2 \\
\leq (1 + \delta) \left( \beta_2^2 + \beta_3^2 \right) \left( \| \phi_x \|_B^2 + \| \phi_z \|_B^2 \right) + \left( 1 + \frac{1}{\delta} \right) \| \alpha \phi_x + q \|_B^2.
\begin{equation}
(6.11)
\end{equation}

Next, since \( \beta_2^2 + \beta_3^2 < 1 \), \( \delta \) can be chosen such that \( (1 + \delta)(\beta_2^2 + \beta_3^2) \leq (1 - \delta) \). Therefore, by (6.10),
\[
\delta(\| \phi_x \|_B^2 + \| \phi_z \|_B^2) \leq \left( 1 + \frac{1}{\delta} \right) \| \alpha \Phi_x + q \|_B^2 + \| \phi_x \|_B^2 + \| \phi_z \|_B^2 + 2 \partial_t (\Phi_x, \Phi_t) - 2(\Phi_t, F).
\]

Since \( (\Phi_x, \Phi_t) \) can be estimated by \( E \), there follows
\begin{lemma}
\begin{align*}
\int_0^T \left( \| \phi_x \|_B^2 + \| \phi_z \|_B^2 + \| \phi_t \|_B^2 + \| \phi_z \|_B^2 \right) \, dt \\
\leq \text{const}(E(0)) + \int_0^T \| F \|_B^2 \, dt + \int_0^T \| q \|_B^2 \, dt.
\end{align*}
\end{lemma}

An estimate for \( \Phi \) itself can easily be obtained by the change of variable \( \Phi \to e^{it} \Phi \), as described in section 6.1.2 or in appendix 1 of [18]. Together with the results of lemmas 1 and 2, this establishes \( \Box \)

\begin{theorem}
The IBVP (6.1)–(6.4) is strongly well-posed in the sense of (6.5).
\end{theorem}

The result can also be generalized to half-plane problems for wave equations of the general constant coefficient form
\[
\Phi_{tt} = 2b^i \Phi_{x^i} + h^{ij} \Phi_{x^j}, \quad x_1 \geq 0, \quad -\infty < (y, z) < \infty, \quad x^i = (x, y, z),
\begin{equation}
(6.12)
\end{equation}
where $h^{ij}$ is a metric of $(++++)$ signature. By coordinate transformation, $(6.12)$ can be transformed into $(6.1)$ and the appropriate boundary conditions formulated. See [18] for details.

This example illustrates from the PDE perspective the constructions necessary to establish strong well-posedness. For the purpose of establishing the strong well-posedness of the IBVP for the wave equation on a general curved-space background, it is also instructive to take advantage of the geometric nature of the problem.

In terms of standard relativistic notation, consider the wave equation

$$g^{ab} \nabla_a \nabla_b \Phi = F$$  \hspace{1cm} (6.13)

for a massless scalar field propagating on a Lorentzian spacetime $M$ foliated by compact, three-dimensional time-slices $S_t$, with boundary $T$ foliated by $B_t$. Here $\nabla$ denotes the covariant derivative associated with the spacetime metric $g^{ab}$. For notational simplicity, let $\Phi_a = \nabla_a \Phi$.

The IBVP consists in finding solutions of $(6.13)$ subject to the initial Cauchy data

$$\Phi|_{S_0} = f_1, \quad n^b \Phi_b|_{S_0} = f_2$$ \hspace{1cm} (6.14)

and the boundary condition

$$[(T^b + aN^b) \Phi_b]_T = q,$$ \hspace{1cm} (6.15)

with data $q$ on $T$. Here $n^b$ is the future-directed unit normal to the time-slices $S_t$ and $N^b$ is the outward unit normal to $T$; $T^b$ is an arbitrary future-directed timelike vector field which is tangent to $T$ and $a > 0$. The motion of the boundary is described geometrically by the hyperbolic angle $\tan \Theta = N^b n_b$. Without loss of generality, assume the normalization $g_{ab} T^b T^c = -1$. A Sommerfeld boundary condition then corresponds to the choice $a = 1$ for which $T^b + N^b$ points in an outgoing null direction.

In order to establish estimates, consider the energy–momentum tensor of the scalar field

$$\Theta_b^a = \Phi_b \Phi^a - \frac{1}{2} \delta_b^a \Phi^\nu \Phi_\nu.$$  

The essential idea is the use of an energy associated with a timelike vector $u^a = T^a + \delta N^a$, where $0 < \delta < 1$, so that $u^a$ points outward from the boundary. The corresponding energy $E(t)$ and the energy flux $P(t)$ through $B_t$ are

$$E(t) = \int_{S_t} u^b \Theta_b^a n_a,$$  \hspace{1cm} (6.16)

which is a covariant version of the non-standard energy $(6.6)$, and

$$P(t) = \int_{B_t} u^b \Theta_b^a N_a.$$  \hspace{1cm} (6.17)

It follows from the timelike property of $u^a$ that $E(t)$ is a norm for $\Phi_a(t)$.

Energy conservation for the scalar field, i.e. integration by parts, gives

$$\partial_t E = P - \int_{S_t} (\Theta_{ab} \nabla_b u^a + u^a \Phi_a F),$$

so that

$$\partial_t E \leq P + \text{const} \left( E + \int_{S_t} F^2 \right).$$  \hspace{1cm} (6.18)

The required estimates arise from an identity satisfied by the flux density

$$u^a \Theta_b^a N_a = -\frac{\delta}{2} \left( (N^a \Phi_a)^2 + (T^a \Phi_a)^2 + Q^{ab} \Phi_a \Phi_b + N^a \Phi_a T^b \Phi_b + \delta (N^a \Phi_a)^2 + \delta (T^a \Phi_a)^2 \right)$$  \hspace{1cm} (6.19)
where $Q_{bc} = g_{bc} + T_b T_c - N_b N_c$ is the positive-definite 2-metric in the tangent space of the boundary orthogonal to $T^a$. By using the boundary condition to eliminate $T^a \Phi_a$ in the last group of terms, there follows

$$
\begin{aligned}
\theta^b \partial_a N_a &= \frac{\delta}{2} \left( (N^a \Phi_a)^2 + (T^a \Phi_a)^2 + Q_{ab} \Phi_a \Phi_b + (a + \delta(1 + a^2)) (N^a \Phi_a)^2 \right) \\
&\quad + (1 - 2a \delta) N^a \Phi_a q + \delta q^2 \\
&= -\frac{\delta}{2} \left( (N^a \Phi_a)^2 + (T^a \Phi_a)^2 + Q_{ab} \Phi_a \Phi_b - (a - \delta(1 + a^2)) \right) \\
&\quad \times \left( N^a \Phi_a - \frac{(1 - 2a \delta) q}{2 (a - \delta(1 + a^2))} \right)^2 + \left( \delta + \frac{(1 - 2a \delta)^2}{4 (a - \delta(1 + a^2))} \right) q^2.
\end{aligned}
$$

The choice

$$0 < \delta < \frac{a}{1 + a^2}$$

(which also guarantees that $\delta < 1$ so that $\theta^a$ is timelike) gives the inequality

$$
\theta^b \partial_a N_a \leq -\frac{\delta}{2} \left( (N^a \Phi_a)^2 + (T^a \Phi_a)^2 + Q_{ab} \Phi_a \Phi_b \right) + \text{const} q^2.
$$

It now follows from (6.18) and (6.20) that

$$
\partial_t E + \int_{S_t} \frac{\delta}{2} \left( (N^a \Phi_a)^2 + (T^a \Phi_a)^2 + Q_{ab} \Phi_a \Phi_b \right) \\
\leq \text{const} \left( E + \int_{S_t} F^2 + \int_{S_t} q^2 \right)
$$

This is the required estimate of the gradient $\Phi_a$ on the boundary (as well as the usual estimate of the energy $E$) to prove that the problem is strongly well-posed. As in the previous example, an estimate of $\Phi$ itself follows from the change of variable $\Phi \to e^{\mu \Phi}$, which introduces a mass term in (6.13).

6.1.2. The quasilinear case. Estimate (6.21) is sufficient to establish criterion (6.5) for strong well-posedness of the IBVP for the linear wave equation with constant metric coefficients. In order to extend the result to the quasilinear case on a curved-space background, where the metric depends upon $\Phi$ and $\Phi_a$, it is necessary to show that the corresponding estimates hold for arbitrarily high derivatives of $\Phi$. In the process, this also requires stability of the system under the addition of lower differential order terms, which arise under the differentiation of the wave equation. These requirements are sometimes neglected or misunderstood in the relativity literature.

More generally, local existence theorems for variable coefficient or quasilinear equations follow by iteration of solutions of the linearized equations with frozen coefficients. The energy estimates for the frozen coefficient problem establish the existence of a unique solution which depends continuously on the data. The extension of this result to the quasilinear case first requires that the problem with variable coefficients be strongly well-posed. For this, it is already necessary to obtain estimates for arbitrarily high derivatives of the solution to the linearized problem.

For the purpose of illustrating the procedure, it suffices to consider the IBVP for the two(spatial)-dimensional wave equation with variable coefficients,

$$
\Phi_{tt} = P \Phi + R \Phi + F, \quad x \geq 0, \quad -\infty < y < \infty,
$$

with smooth initial data

$$
\Phi = f_1, \quad \Phi_t = f_2, \quad t = 0,
$$

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and the boundary condition
\[
\alpha(t,y)\Phi_t = \Phi_x - \mu \Phi + r(t,y)\Phi + q(t,y), \quad \alpha(t,y) \geq \text{const} > 0, \quad \mu = \text{const} > 0
\]  
(6.24)

with smooth, compatible boundary data \( q \). Here
\[
P\Phi = (a\Phi_x)_x + (b\Phi_y)_y - 2\mu \Phi_t - \mu^2 \Phi, \quad a > a_0 = \text{const} > 0, \quad b > b_0 = \text{const} > 0,
\]
is an elliptic operator which has been modified by terms which arise in (6.22) by the transformation \( \Phi \rightarrow e^{\omega t} \Phi \), where \( \mu \) introduces a mass term and
\[
R \Phi = c_1 \Phi_x + c_2 \Phi_y + c_3 \Phi_x + c_4 \Phi
\]
are terms of lower (zeroth and first) differential order. The coefficients \( a, b \) and \( c_i \) are smooth functions of \((t,x,y)\).

Consider the norm for the Cauchy data
\[
E = \|\Phi\|_{2}^2 + (\Phi_x, a\Phi_x) + (\Phi_y, b\Phi_y) + \mu^2 \|\Phi\|_{2}^2.
\]
Integration by parts leads to
\[
\partial_t E = -4\mu \|\Phi\|_{2}^2 + 2(\Phi_t, F) + 2(\Phi_t, R \Phi) - 2(\Phi_t, a\Phi_x)_x + (\Phi_t, a\Phi_x)_x + (b\Phi_y, \Phi_y)
\leq \text{const} \|F\|_{2}^2 + E - 2(\Phi_t, a\Phi_x)_x. 
\]  
(6.25)

The boundary condition gives
\[
- (\Phi_t, a\Phi_x)_x = - (\Phi_t, a\Phi_x)_x - \mu (\Phi_t, a\Phi)_y + (\Phi_t, a\phi \Phi + aq)_y
= - (\Phi_t, a\Phi_x)_x - \mu (\Phi_t, a\phi \Phi)_y - \mu (\Phi_t, (a - a_0)\Phi)_y + (\Phi_t, a\phi \Phi + aq)_y
\leq - \frac{1}{2} \mu a_0 \partial_x \|\Phi\|_{2}^2 - \frac{1}{2} (\Phi_t, a\phi \Phi)_y + \text{const} \|F\|_{2}^2 + \|q\|_{2}^2.
\]  
(6.26)

Therefore, from (6.25),
\[
\partial_t (E + \mu a_0 \|\Phi\|_{2}^2) + (\Phi_t, a\phi \Phi)_y
\leq \text{const} \left( E + \|\Phi\|_{2}^2 + \|F\|_{2}^2 + \|q\|_{2}^2 \right).
\]  
(6.27)

This establishes that the energy estimate is stable against lower order perturbations. Now it is possible to estimate the derivatives. For the derivatives \( Y = \Phi_x \) and \( T = \Phi_t \) tangential to the boundary, differentiatition of the wave equation gives
\[
Y_{tt} = PY + RY + R_3 \Phi + (a\Phi_x)_x + (b\Phi_y)_y + F_y 
\]  
(6.30)
\[
T_{tt} = PT + RT + R_3 \Phi + (a\Phi_x)_x + (b\Phi_y)_y + F_t.
\]  
(6.31)

Here \( R, \Phi \) and \( R_3 \Phi \) are linear combinations of first derivatives of \( \Phi \) which have already been estimated and can be considered part of the forcing term \( F \). Also, the wave equation (6.22) implies
\[
a\Phi_{xx} = T_t - bY_x + \text{terms that have already been estimated},
\]
so that \( \Phi_{xx} \) is also lower order with respect to (6.30) and (6.31). Thus, except for lower order terms, \( Y \) and \( T \) solve the same wave equations (6.30) and (6.31) as \( \Phi \), with the same boundary conditions up to lower order terms. Therefore, all second derivatives \( \Phi_{xy} \) and \( \Phi_{tt} \) can be estimated as well as \( \Phi_{xx} \). Repetition of this process gives estimates for any number of derivatives.
In order now to show the existence of a solution to the variable coefficient problem, one approach, which is particularly familiar to numerical relativists, is to approximate the PDE by a stable finite-difference approximation. This approach is detailed in [43] where summation by parts (SBP) is applied to the finite-difference problem in the analogous way that integration by parts is used above in the analytic problem. The SBP approach shows that the corresponding estimates hold independently of grid size. The existence of a solution of the analytic problem then follows from the limit of vanishing grid size.

It also follows from the estimates for arbitrary derivatives of the variable coefficient problem that Sobolev’s theorems can be used to establish similar, although local in time, estimates for quasilinear systems. Then the same iterative methods used for first-order symmetric hyperbolic systems can be used to show that well-posedness extends locally in time to the quasilinear case. In this way, it was shown in [18] that the general quasilinear wave problem (6.13)–(6.15), where the spacetime metric now depends upon $\Phi$ and $\Phi_\alpha$, is strongly well-posed.

6.1.3. Systems of wave equations. The strong well-posedness of the IBVP for the quasilinear scalar wave (6.13)–(6.15) can be generalized to a system of coupled wave equations

$$g^{ab}(\Phi) \nabla_a \nabla_b \Phi^A = F^B(\Phi, \nabla \Phi), \quad A = 1, 2, ..., N, \quad (6.32)$$

with smooth initial data

$$\Phi^A \bigg|_{S_0} = f^A_1, \quad n^b \nabla_b \Phi^A \bigg|_{S_0} = f^A_2, \quad (6.33)$$

and the boundary condition

$$(T^b + \alpha N^b) \nabla_b \Phi^A \bigg|_T = c^{aA}_B \nabla_a \Phi^B \bigg|_T + d^A_B \Phi^B \bigg|_T + q^A, \quad (6.34)$$

where $a = a(x, \Phi) > 0$, $q^A = q^A(x)$, $c^{aA}_B = c^{aA}_B(x, \Phi)$ and $d^A_B = d^A_B(x, \Phi)$ are smooth functions of their arguments. All data are compatible. As before, each time-slice $S_t$ is spacelike, with future-directed unit normal $n^b(x, \Phi)$; the boundary $T$ is timelike with outward unit normal $N^a(x, \Phi)$ and $T^a = T^a(x, \Phi)$ is an arbitrary future-directed timelike vector field tangent to $T$.

In [19], it was shown that the IBVP (6.32)–(6.34) is strongly well-posed given certain restrictions on $c^{aA}_B$, i.e. there exists a solution locally in time which satisfies (6.5) in terms of the corresponding $L_2$ norms for $\Phi^A$ and its gradient. One important situation in which the restrictions on $c^{aA}_B$ are satisfied is when it can be transformed into the upper diagonal form

$$c^{aA}_B = 0, \quad B < A.$$  

This has important applications to the constrained systems of wave equations obtained by formulating Maxwell’s equations in the Lorentz gauge or Einstein’s equations in the harmonic gauge [19], as discussed in section 10.

6.1.4. Pseudo-differential theory. The previous scalar-wave problems required a non-standard energy to obtain the necessary estimates. In more general problems, an effective choice of energy might not be obvious or even exist. Pseudo-differential theory provides an alternative treatment of such cases. The approach is based upon a Fourier transform for the spatial dependence and a Laplace transform in time. It can be applied equally well to first- or second-order systems. Here I illustrate how it applies to the second-order wave equation. The more general theory for a system of equations is usually presented in first-order form and is reviewed in section 6.2.1.

As an illustrative example, consider the two(spatial)-dimensional version of the IBVP for the scalar wave considered in section 6.1.1,

$$\Phi_{tt} = \Phi_{xx} + \Phi_{yy} + F, \quad x \geq 0, \quad -\infty < y < \infty, \quad (6.35)$$
with boundary condition at \( x = 0 \)
\[
\Phi_t - \alpha \Phi_x - \beta \Phi_y = q, \quad \alpha > 0, \quad |\beta| < 1,
\]
(6.36)
with compact boundary data \( q \) and initial data
\[
\Phi(0, x, y) = f_1(x, y), \quad \Phi_t(0, x, y) = f_2(x, y).
\]
(6.37)
The following simple observation reveals the underlying idea. The system cannot be well-posed if the homogeneous version of (6.35)–(6.37) with \( F = q = 0 \) admits arbitrarily fast-growing solutions. The homogeneous system has solutions of the form
\[
\Phi_1(t, x, y) = e^{st} \Phi_1(x) - s \Phi_1(0, x), \quad |\Phi_1|_\infty < \infty,
\]
(6.38)
where
\[
\varphi_{xx} - (s^2 + \omega^2) \varphi = 0, \quad s \varphi(0) = \alpha \Phi_1(0, x) + i \beta \omega \varphi(0).
\]
(6.39)
Here \( \varphi(x) \) is a smooth bounded function, so that its maximum norm \( |\varphi|_\infty \) is finite, \( \omega \) is a real constant and \( s = \eta + i \xi \) a complex constant. This poses an eigenvalue problem. If there are solutions with \( \Re s > 0 \), then
\[
\Phi_\nu = e^{\nu t + i \omega \xi \eta} \varphi(\nu x)
\]
is also a solution for any \( \nu > 0 \), so that there are solutions which grow arbitrarily fast exponentially. Therefore, a necessary condition for a well-posed problem is that solutions with \( \Re s > 0 \) must be ruled out by the boundary condition.

The general solution of the ordinary differential equation (6.39) is
\[
\varphi = \sigma_1 e^{\kappa_+ x} + \sigma_2 e^{\kappa_- x},
\]
(6.41)
where
\[
\kappa_{\pm} = \pm \sqrt{s^2 + \omega^2}
\]
solve the characteristic equation
\[
\kappa^2 - (s^2 + \omega^2) = 0.
\]
(6.42)
Here \( \Re \kappa_+ > 0 \) and \( \Re \kappa_- < 0 \) for \( \Re s > 0 \). By assumption, \( \varphi \) is bounded which requires that \( \sigma_1 = 0 \), i.e.
\[
\varphi = \sigma_2 e^{\kappa_- x}.
\]
(6.43)
Introducing (6.43) into the boundary condition (6.40) gives
\[
(s - \alpha \kappa_- - i \beta \omega) \sigma_2 = 0.
\]
(6.44)
Since \( \Re \kappa_- < 0 \) and by assumption \( \alpha > 0 \), there are no solutions with \( \Re s > 0 \). Thus, this necessary condition for a well-posed problem is satisfied.

In order to proceed further, it is technically convenient to assume that the initial data (6.37) vanish. This may always be achieved by the transformation
\[
\Phi \to \Phi - e^{-t} f_1 - te^{-t} (f_2 + f_1),
\]
(6.45)
so that the initial data get swept into the forcing term \( F \). Then (6.35)–(6.37) can be solved by the Fourier transform with respect to \( y \) and the Laplace transform with respect to \( t \), i.e. in terms of
\[
\hat{\Phi}(s, x, \omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dy e^{i \omega y} \int_{0}^{\infty} dt e^{-st} \Phi(t, x, y), \quad \Re s > 0,
\]
(6.46)
where \( \omega \) is real and \( s \) is complex. The inhomogeneous versions of (6.39) and (6.40) imply that the coefficients satisfy
\[
\hat{\Phi}_{xx} - (s^2 + \alpha^2) \hat{\Phi} = -\hat{F}
\]
\[
(s - i\beta \omega) \hat{\Phi}(s, 0, \omega) - \alpha \hat{\Phi}_x(s, 0, \omega) = \hat{q}(s, \omega).
\]

(6.47)

Since it has already been shown that the homogeneous system (6.39)–(6.40) has no eigenvalues for \( \Re s > 0 \) and \( \Re \kappa < 0 \), it follows that (6.47) has a unique solution \( \hat{\Phi} \). Inversion of the Fourier–Laplace transform then gives a unique solution for \( \Phi \).

The well-posedness of a variable coefficient or quasilinear wave problem also requires estimates of the higher derivatives of \( \Phi \). The system of equations for the derivatives is obtained by differentiating the wave equation and the boundary condition. In that process, any variable coefficient terms in the boundary condition lead to inhomogeneous boundary data for the derivatives. It is possible to transform the boundary data \( q \) to 0 by a transformation analogous to (6.45), which sweeps \( q \) and its derivatives into the forcing term \( F \). If these inhomogeneous boundary data are continually subtracted out of the boundary condition, inhomogeneous terms of higher differential order appear in the forcing term. As a consequence, the resulting estimates would bound lower derivatives of the solution in terms of higher derivatives of the data, a process referred to as 'losing' derivatives.

Instead, a different approach is necessary to establish well-posedness. It is simple to calculate the solution for \( \hat{F} = 0 \). Corresponding to (6.43) and (6.44), there follows
\[
\hat{\Phi}(s, x, \omega) = e^{s \cdot \tau} \hat{\Phi}(s, 0, \omega),
\]
where
\[
(s - \alpha \kappa - i\beta \omega) \hat{\Phi}(s, 0, \omega) = \hat{q}(s, \omega).
\]

(6.48)

It is now possible to establish [17]

**Boundary stability.** Solution (6.48) satisfies the estimates
\[
\begin{align*}
|\hat{\Phi}_x(s, 0, \omega)| &\leq K|\hat{q}(s, \omega)|, \\
|\hat{\Phi}(s, 0, \omega)| &\leq K|\hat{q}(s, \omega)|,
\end{align*}
\]

(6.49)

where the constant \( K \) is independent of \( s \) and \( \omega \). Similar estimates hold for all the derivatives.

Estimates (6.49) follow from purely algebraic consequences of the eigenvalue relations (6.42) and (6.44). The essential steps are to show that

1. there is a constant \( \delta_1 > 0 \) such that \( |\Re \kappa| > \delta_1 |\Re s| \);
2. for all \( \omega \) and \( s \) with \( \Re s \geq 0 \), there is a constant \( \delta_2 > 0 \) such that \( |s - \alpha \kappa - i\beta \omega| \geq \delta_2 |s|^2 + |\omega|^2 \).

See [17] for the details.

Boundary stability allows the application of the theory of pseudo-differential operators to show that the IBVP is strongly well-posed in the generalized sense,
\[
\int_0^T \|\Phi(t)\|^2\,dt + \int_0^T \|\Phi(t)\|^2\,dt \leq K_T \left( \int_0^T \|F(t)\|^2\,dt + \int_0^T \|q(t)\|^2\,dt \right), \quad 0 \leq t \leq T,
\]

(6.50)

where \( \Phi = (\Phi_x, \Phi_{xx}) \).

The theory is discussed in section 6.2.1 in the standard context of first-order systems. But the first-order theory is flexible enough to apply to second-order systems. In particular, in section 6.2.1 it is applied to show that the IBVP for the quasilinear version of the second-order wave equation with boundary condition (6.35)–(6.36) is well-posed in the generalized sense.
Strong well-posedness in the generalized sense is similar to strong well-posedness (6.5) except now the initial data have been swept into the forcing term and the estimate for $\Phi$ in the interior involves a time integral. In both cases, the gradients at the boundary are estimated by the boundary data and the forcing, i.e. a derivative is gained at the boundary. This ensures that the well-posedness of the local half-plane problem can be extended globally to include boundaries that lead to multiple reflections.

6.1.5. Generalized eigenvalues. Strong well-posedness in the generalized sense not only rules out the eigenvalues of (6.40) with $\eta = \Re(s) > 0$ but also generalized eigenvalues for which $\eta = 0$. This is implicit in the estimates for boundary stability (6.49) in which the constant $K$ is independent of $s$. However, generalized eigenvalues can exist in well-behaved physical systems. A prime example is a surface wave which travels tangential to the boundary with periodic time dependence. See [15] for the treatment of such an example from Maxwell theory.

Generalized eigenvalues are ruled out by the boundary conditions required for strong well-posedness in the generalized sense and historically have been treated on an individual basis. However, a new approach to this problem has recently been formulated by Kreiss [47]. This approach splits the problem into two subproblems:

(1) one in which the forcing vanishes, $F = 0$
(2) one in which the boundary data are homogeneous, $q = 0$

A second-order wave problem is called well-posed in the generalized sense if these subproblems satisfy the corresponding estimates

$$\int_0^t \|\Phi(\tau)\|_B^2 d\tau \leq K_T \int_0^t \|q(\tau)\|_B^2 d\tau, \quad 0 \leq t \leq T, \quad (6.51)$$

$$\int_0^t \|\Phi(\tau)\|_B^2 d\tau \leq K_T \int_0^t \|F(\tau)\|_B^2 d\tau, \quad 0 \leq t \leq T. \quad (6.52)$$

Here it is only required that $\Phi$, and not its gradient $\Phi$, be estimated by the boundary data $q$. Thus, the solution no longer gains a derivative at the boundary. However, no global problems arise from multiple reflections because estimate (6.52) implies the gain of one derivative in the interior.

As examples, consider the scalar-wave problem (6.35) with the two choices of boundary conditions at $x = 0$,

(A) $\Phi_x - i\beta \Phi_y = q$,

(B) $\Phi_x - \beta \Phi_y = q$,

where $\beta$ is real, with $|\beta| < 1$. In case (A), $\Phi$ is complex. Introducing these boundary conditions into the homogeneous system (6.38)–(6.40) gives

(A) $\kappa = \omega \beta$,

(B) $\kappa = -\omega \beta$,

with $\kappa^2 = \omega^2 - \alpha^2$.

In neither case is there a solution with $\Re s > 0$ but both cases possess generalized eigenvalues,

(A) $s^2 = -\alpha^2(1 - \beta^2), \quad \Re s = 0$,

(B) $s^2 = -\alpha^2(1 + \beta^2), \quad \Re s = 0$.

The corresponding eigenfunctions are the surface waves

$$e^{i\omega(\pm\sqrt{1-\beta^2} + 1) - \omega \beta \tau} x, \quad (6.53)$$
and the oscillatory waves

\[ e^{i\omega(\pm\sqrt{1+\beta^2t^2+\beta x+y})}, \]

(6.54)

which give rise to glancing waves for \( \beta = 0 \). By investigating the inhomogeneous problem, it can be shown that both choices of boundary condition give rise to an IBVP which satisfies (6.51) and (6.52) and is well-posed in the generalized sense [47].

6.2. First-order symmetric hyperbolic systems

Most of the work on the IBVP for hyperbolic systems has been directed toward fluid dynamics, where a first-order formulation is natural. Here I describe the essentials of the two main approaches, pseudo-differential theory and the theory of symmetric hyperbolic systems.

6.2.1. Pseudo-differential theory. In order to summarize the pseudo-differential theory for a first-order symmetric hyperbolic system, consider first the constant coefficient system

\[ u_t = \mathcal{P}(\partial_x)u + F, \quad \mathcal{P}(\partial_x) = \mathcal{P}'\partial_{x_1} + \sum_{j=2}^{m} B_j \partial_{x_j} \]

(6.55)

on the half-space

\[ t \geq 0, \quad x_1 \geq 0, \quad -\infty < x_j < \infty, \quad j = 2, \ldots, m, \]

with initial data

\[ u(0, x) = f(x). \]

(6.56)

Here \( u(t, x) = (u^{(1)}(t, x), \ldots, u^{(N)}(t, x)) \) is a vector-valued function of the real variables \((t, x) = (t, x_1, \ldots, x_m)\) and \( A, B_j \) are constant \( N \times N \) matrices. In applications to spacetime, \( m = 3 \) but the number of spatial dimensions does not complicate the theory. The notations \( \langle u, v \rangle \) and \( |u|^2 = \langle u, u \rangle \) denote the inner product and norm in the \( N \)-dimensional linear space. All data are smooth, compatible and have compact support.

The symbol representing the principal part of the system,

\[ \mathcal{P}(i\omega) = iA\omega_1 + iB(\omega-), \quad B(\omega-) = \sum_{j=2}^{m} B_j \omega_j \quad |\omega| = 1, \]

(6.57)

is obtained by replacing \( \partial_x \) by its Fourier representation \( i\omega = (i\omega_1, i\omega-), \omega- = (\omega_2, \ldots, \omega_m) \). Symmetric hyperbolicity requires that \( A \) and \( B \) be self-adjoint matrices so that the eigenvectors of \( \mathcal{P} \) form a complete set with purely imaginary eigenvalues for all real \( \omega \). More precisely, there exists a symmetric, positive-definite symmetrizer \( H \) such that \( HA \) and \( HB_j \) are self-adjoint. See [48] for more general applications.

Here it is also assumed that the boundary matrix \( A \) is non-singular so that it can be transformed into the form

\[ A = \begin{pmatrix} -\Lambda^I & 0 \\ 0 & \Lambda^I \end{pmatrix}, \]

(6.58)

where \( \Lambda^I, \Lambda^H \) are real positive-definite diagonal matrices acting on the \( P \)-dimensional subspace \( u^I \) and the \((N-P)\)-dimensional subspace \( u^H \), respectively. The theory also applies to the singular case where the boundary is uniformly characteristic, i.e. the kernel of \( A \) has constant dimension [49]. See section 6.2.2 for a treatment of the singular case by the energy method.
The IBVP requires $P$ boundary conditions at $x_1 = 0$, corresponding to the $P$ ingoing modes in the plane wave decomposition carried out below in conjunction with (6.61) and (6.64). They are prescribed in the form
\[ u'(t, 0, x_\sigma) = Su(t, 0, x_\sigma) + q(t, x_\sigma), \quad x_\sigma = (x_2, \ldots, x_m). \tag{6.59} \]

The main ingredient of a definition of well-posedness is the estimate of the solution in terms of the data. See section 7.3 of [43]. By a transformation analogous to (6.45), the IBVP (6.55), (6.56), (6.59) reduces to a problem with homogeneous initial data $f = 0$. The required estimate is the first-order version of estimate (6.50) for the second-order wave equation. The first-order problem is called \textit{strongly well-posed in the generalized sense} if there is a unique solution $u$ such that
\[ \int_0^t \|u(\tau)\|^2 d\tau + \int_0^t \|u(\tau)\|_{L_\sigma}^2 d\tau \leq K_T \left( \int_0^t \|F(\tau)\|^2 d\tau + \int_0^t \|q(\tau)\|_{L_\sigma}^2 d\tau \right), \quad 0 \leq t \leq T, \tag{6.60} \]
where the constant $K_T$ does not depend on $F$ or $q$. Here $\|u\|$ and $\|u\|_{L_\sigma}$ are the $L_2$ norms of $|u|$ over the half-space and the boundary, respectively.

As for the scalar-wave problem considered in section 6.1.4, the IBVP is not well-posed if the homogeneous system $F = q = 0$ admits wave solutions
\[ u(t, x_1, x_\sigma) = e^{\kappa t + i(\omega_\sigma \cdot x_\sigma)} \varphi(x_1), \quad \langle \omega, x_\sigma \rangle = \sum_{j=2}^m \omega_j x_j, \quad \Re s > 0, \tag{6.61} \]
with $|\varphi|_\infty < \infty$. The existence of such homogeneous solutions would imply the existence of solutions which grow arbitrarily fast exponentially.

In order to decide whether such homogeneous waves exist, introduce (6.61) into (6.55) and (6.59) to obtain
\[ s \varphi = \lambda \varphi_{x_1} + iB(\omega_\sigma) \varphi, \quad x_1 \geq 0, \]
\[ \varphi'(0) = S \varphi_I(0), \quad |\varphi|_\infty < \infty. \tag{6.62} \]
This is an eigenvalue problem for a system of ordinary differential equations which can be solved in the usual way. Let $\kappa$ denote the solutions of the characteristic equation
\[ \operatorname{Det}[\lambda I - (sl - iB(\omega_\sigma))] = 0, \tag{6.63} \]
obtained by setting $\varphi(x_1) = e^{\kappa x_1} \varphi(0)$.

It can be shown that
\begin{enumerate}
  \item there are exactly $r$ eigenvalues with $\Re \kappa < 0$ and $n - r$ eigenvalues with $\Re \kappa > 0$;
  \item there is a constant $\delta > 0$ such that, for all $s$ with real $\Re s > 0$ and all $\omega_\sigma$,
  \[ |\Re \kappa| > \delta \Re s. \]
\end{enumerate}
In particular, for $\Re s > 0$, there are no $\kappa$ with $\Re \kappa = 0$.

See [46] for the proof.

If all eigenvalues $\kappa_j$ are distinct, the general solution of (6.62) has the form
\[ \varphi = \sum_{\Re \kappa_j < 0} \sigma_j e^{\kappa_j x_1} h_j + \sum_{\Re \kappa_j > 0} \sigma_j e^{\kappa_j x_1} h_j, \tag{6.64} \]
where $h_j$ are the corresponding eigenvectors. (If the eigenvalues are degenerate, the usual modifications apply.) For bounded solutions, all $\sigma_j$ in the second term are zero. Introducing $\varphi$ into the boundary conditions (6.62) at $x_1 = 0$ gives a linear system of $r$ equations for the $r$ unknowns $(\sigma_1, \ldots, \sigma_r) \equiv \sigma$ of the form
\[ C(s, \omega_\sigma) \sigma = 0. \tag{6.65} \]
Therefore, the problem is not well-posed if for some $\omega$ there is an eigenvalue $s_0$ with $\Re s_0 > 0$, i.e. $\det C(s_0, \omega) = 0$. In that case, the linear system (6.65), and therefore also (6.62), has a nontrivial solution. Thus, the determinant condition

$$\det C(s_0, \omega) \neq 0, \quad \Re s_0 > 0,$$

is necessary for a well-posed problem.

Thus, in order to consider a well-posed problem, assume that $\det C \neq 0$ or $\Re s > 0$. Then the inhomogeneous IBVP (6.55), (6.56), (6.59) can be solved by the Laplace transform in time and the Fourier transform in the tangential variables. Again set $u(0, x) = f(x) = 0$.

Then

$$s\hat{u} = A\hat{u}_x + iB(\omega)\hat{u} + \hat{F},$$

$$\hat{u}'(0) = \hat{S}\hat{u}^{\mathrm{II}}(0) + \hat{q}. \quad (6.67)$$

Since, by assumption, (6.62) has only the trivial solution for $\Re s > 0$, (6.68) has a unique solution. Inverting the Fourier and Laplace transforms gives the solution in physical space.

As in the scalar-wave case, it is simple to solve (6.67) for $\hat{F} = 0$. From the inhomogeneous versions of (6.64) and (6.65),

$$\hat{u}(s, x_1, \omega) = \sum_{\Re \kappa < 0} \sigma_j e^{\kappa x_1} h_j,$$

where the $\sigma_j$ are determined by

$$C(s, \omega) \sigma = \hat{q}.$$

It is now possible to establish the pseudo-differential version of boundary stability:

for all $\omega, s$ with $\Re s > 0$, there is a constant $K$ independent of $\omega, s$ and $\hat{q}$ such that the solutions of (6.67) and (6.68) with $\hat{F} = 0$ satisfy

$$|\hat{u}(s, 0, \omega)| \leq K|\hat{q}(s, \omega)|. \quad (6.69)$$

Boundary stability is equivalent to the requirement that the eigenvalue problem (6.62) has no eigenvalues for $\Re s \geq 0$ or that $\det C(\omega, s) \neq 0$ for $\Re s \geq 0$. In particular, it rules out generalized eigenvalues. It is essential to establish the following.

**Main Theorem:** If the half-space problem is boundary stable, then it is strongly well-posed in the generalized sense of (6.60).

See [46] for the proof, where boundary stability is used to construct a symmetrizer in the Fourier–Laplace representation which leads to the estimate

$$\eta \|\hat{u}(s, x_1, \omega)\|^2 + |\hat{u}(s, 0, \omega)|^2 \leq \text{const} \left(\frac{1}{\eta} \|\hat{F}\|^2 + c|\hat{q}|^2\right). \quad (6.70)$$

Inversion of the Fourier–Laplace transform proves the theorem.

The pseudo-differential theory has far-reaching consequences. In particular, the computational rules for pseudo-differential operators imply the following.

1. The Laplace transform only requires that the estimates hold for $\eta > \eta_0 > 0$, where $\eta_0$ is sufficiently large to allow for (controlled) exponential growth due to lower order terms.
   This is essential for extending strong well-posedness to systems with variable coefficients.
2. Boundary stability is also valid if the symbol depends smoothly on $(t, x)$ and is not destroyed by lower order terms. Therefore, the problem can be localized and well-posedness in general domains can be reduced to the study of the Cauchy problem and half-space problems.
The principle of frozen coefficients holds. The properties of the pseudo-differential operators give rise to estimates of derivatives in the same way as for standard PDEs. Therefore, strong well-posedness in the generalized sense can be extended to linear problems with variable coefficients and, locally in time, to quasilinear problems.

Since pseudo-differential operators are much more flexible than standard differential operators, they can be applied to second-order systems as well as first-order systems. Consider, for example, problem (6.35)–(6.37) discussed in section 6.1.4. After transforming the initial data to zero, the Fourier–Laplace transform becomes

\[ \hat{\Phi}_{xx} = (s^2 + \omega^2) \hat{\Phi} - \hat{F}, \]
\[ s\hat{\Phi} - \alpha \hat{\Phi}_x - i\beta \omega \hat{\Phi} = \hat{\eta}. \]  

(6.71)

Introduction of a new variable \( \hat{\Phi}_1 = \sqrt{|s|^2 + \omega^2} \hat{\Psi} \) gives the first-order system

\[ \hat{u}_t = \frac{1}{\sqrt{|s|^2 + \omega^2}} \left( \begin{array}{cc} 0 & |s|^2 + \omega^2 \\ |s|^2 + \omega^2 & 0 \end{array} \right) \hat{u} - \hat{F}, \quad \hat{u} = \left( \begin{array}{c} \hat{\Phi} \\ \hat{\Psi} \end{array} \right), \]
\[ \sqrt{|s|^2 + \omega^2} \hat{\Phi} - \alpha \hat{\Psi} - i\beta \omega \sqrt{|s|^2 + \omega^2} \hat{\Phi} = \hat{\eta}. \]  

(6.72)

where

\[ \hat{F} = \frac{1}{\sqrt{|s|^2 + \omega^2}} \left( \begin{array}{c} 0 \\ \hat{F} \end{array} \right), \quad \hat{\eta} = \frac{1}{\sqrt{|s|^2 + \omega^2}} \hat{\eta}. \]  

(6.73)

The second-order problem (6.35)–(6.37) is strongly well-posed in the generalized sense if the corresponding first-order problem (6.72) with general data \( \hat{F}, \hat{\eta} \) has this property. The second–order version of boundary stability (6.71) established in section 6.1.4, rewritten in terms of the first-order variables, implies

\[ |\hat{\Phi}(s, 0, \omega)| + |\hat{\Psi}(s, 0, \omega)| \leq K |\hat{\eta}(s, \omega)|, \]  

(6.74)

i.e. the first-order version of boundary stability (6.69). Thus, the Main Theorem applies and the second-order problem is strongly well-posed in the generalized sense in the first-order version (6.60), which is equivalent to the second-order version (6.50).

6.2.2. The energy method for first-order symmetric hyperbolic systems. Energy estimates for first-order symmetric hyperbolic systems were first applied to Einstein’s equations in harmonic coordinates by Fischer and Marsden [52] to give an alternative derivation of the results of Choquet–Bruhat for the Cauchy problem. The energy method extends to the quasilinear IBVP with maximally dissipative boundary conditions.

Again, begin by considering the constant coefficient system (6.55)

\[ u_t = P^i \partial_i u + F, \quad P^i \partial_i = A \partial_i + \sum_{j=2}^m B_j \partial_{x_j} \]  

(6.75)

on the half-space

\[ t \geq 0, \quad x_1 \geq 0, \quad -\infty < x_j < \infty, \quad j = 2, \ldots, m, \]

with initial data \( u(0, x) = f(x) \). As before, \( A \) and \( B_j \) are symmetric \( N \times N \) matrices so that the eigenvectors of \( P^i \) form a complete set with real eigenvalues. In matrix notation, there is a symmetric positive-definite symmetrizer \( H_{MN} \) such that \( H_{MN}A^p_q \) and \( H_{MN}B^p_{jk} \) are symmetric.
Here, the boundary matrix $A$ is allowed to be singular, cf [49–51]. With an appropriate choice of symmetrizer, it can be put in the form

$$A = \alpha \begin{pmatrix} -I_P & 0 & 0 \\ 0 & O^Q & 0 \\ 0 & 0 & I_R \end{pmatrix}, \quad \alpha > 0, \quad u = \begin{pmatrix} u^I \\ u^O \\ u^I \end{pmatrix}, \quad (6.76)$$

where $I_P$ and $I_R$ are identity matrices acting on the $P$-dimensional subspace $u^I$ and the $R$-dimensional subspace $u^I$, respectively, and $O^Q$ is a zero matrix acting on the $Q$-dimensional kernel $u^O$, with $N = P + Q + R$. No boundary condition can be imposed on the components of $u^I$, which are the outgoing modes, or the components of $u^O$. The components of $u^O$ satisfy PDEs intrinsic to the boundary. They are referred to as zero-velocity modes since they have no velocity relative to the boundary. As in the discussion of the non-characteristic case in section 6.2.1, there are $P$ ingoing modes and the IBVP requires $P$ boundary conditions at $x_1 = 0$. They are prescribed in the maximal form

$$u^I(t, 0, x) = S u^I(t, 0, x) + q(t, x), \quad x = (x_2, \ldots, x_m), \quad (6.77)$$

where the $P \times R$ matrix $S$ satisfies the dissipative condition that, for homogeneous data $q = 0$, the local energy flux out of the boundary be positive,

$$\mathcal{F} := (u, Au) \geq 0. \quad (6.78)$$

In the simplified form (6.76), this leads to the requirement

$$- |Su^I(t, 0, x)|^2 + |u^I(t, 0, x)|^2 \geq 0, \quad (6.79)$$

where $|u|^2 = (u, u)$ in terms of the linear space inner product.

The rationale for these maximally dissipative boundary conditions results from the energy estimate for the case of homogeneous boundary data $q = 0$. Beginning with

$$\partial_t (u, u) = 2(u, A \partial_t u + \sum_{j=2} B_j \partial_{x_j} u + F), \quad (6.80)$$

integration over the half-space gives

$$\partial_t E := \partial_t \|u\|^2 = 2(u, A \partial_t u) + 2(u, F)$$

$$= - (u, Au) + 2(u, F),$$

$$\leq 2(u, F) \leq \|u\|^2 + \|F\|^2 = E + \|F\|^2, \quad (6.81)$$

where $(u, v)$ denotes the integral of $(u, v)$, etc. Thus, the maximally dissipative boundary conditions provide the required energy estimate. The inhomogeneous boundary data $q$ can be transformed to zero by the change of variable $u \rightarrow u - q$ to obtain an analogous estimate.

More generally, if the boundary is uniformly characteristic so that the kernel of the boundary matrix $A$ has the constant dimension $Q$, then the quasilinear IBVP problem with maximally dissipative boundary conditions is strongly well-posed: a solution exists locally in time which satisfies (6.60). See [53–56, 51] for details.

The theory can also be recast in the covariant spacetime form

$$A^\mu \partial_\nu u = F, \quad (6.82)$$

where $A^\mu = (A^I, A^I)$ are symmetric matrices and $A^I$ is positive definite. As an illustration of this and the various choices of boundary conditions, consider the IBVP for the scalar-wave equation

$$g^{\mu\nu} \partial_\nu \partial_\mu \Phi = 0, \quad x \geq 0, \quad t \geq 0, \quad g^{xx} > 0. \quad (6.83)$$
This can be rewritten in the first-order symmetric hyperbolic form (6.82) for a five-component field $u$ by introducing the auxiliary variables

$$ u = \begin{pmatrix} u_0 \\ u_t \\ u_i \end{pmatrix} = \begin{pmatrix} \Phi \\ \partial_t \Phi \end{pmatrix}. $$

(6.84)

The matrices $A^\mu$ are then given by

$$ A^t = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -g^{tt} & 0 \\ 0 & 0 & g^{ik} \end{pmatrix}, \quad A^i = \begin{pmatrix} 0 & 0 & 0 \\ 0 & -2g^{ij} & -g^{it} \\ 0 & -g^{ij} & 0 \end{pmatrix}, $$

(6.85)

with

$$ F = \begin{pmatrix} u_t \\ 0 \\ 0 \end{pmatrix}. $$

(6.86)

In this first-order form, the Cauchy data consist of $u|_{t=0} = f$ subject to the constraints

$$ C_i := u_i - \partial_i u_0 = 0. $$

(6.87)

The evolution system implies that the constraints satisfy

$$ \partial_t C_i = 0, $$

(6.88)

so that they propagate up the timelike boundary at $x = 0$ and present no complication.

The boundary matrix $(-A^t)$ (oriented in the outward normal direction) has a three-dimensional kernel, whose transposed basis consists of the zero-velocity modes

$$(1, 0, 0, 0, 0), \quad (0, 0, -g^{ty}, g^{tx}, 0) \quad \text{and} \quad (0, 0, -g^{yz}, 0, g^{zy}). $$

(6.89)

In addition, there is one positive eigenvalue and one negative eigenvalue

$$ \lambda_+ = \pm \lambda + g^{tt}, $$

(6.90)

where

$$ \lambda = \sqrt{(g^{tt})^2 + \delta_{ij} g^{ti} g^{tj}}. $$

(6.91)

Thus, precisely one boundary condition is required.

In terms of the normalized eigenvectors,

$$ e_\pm = \frac{1}{\sqrt{\pm 2 \lambda \lambda_\pm}} \begin{pmatrix} 0 \\ \pm \lambda + g^{tt} \\ +g^{tt} \end{pmatrix}, $$

(6.92)

$u = u_+ e_+ + u_- e_-$, where $u_0$ lies in the kernel. The boundary condition takes the form $u_+ - Su_- = q$, subject to the dissipative condition

$$ F = -\langle u, A^t u \rangle \geq 0. $$

(6.93)

For the case of homogeneous data $q = 0$, this requires that

$$ S^2 \leq -\lambda_- / \lambda_+ . $$

(6.94)

The limiting cases $S = \pm \sqrt{-\lambda_- / \lambda_+}$ lead to reflecting boundary conditions. In the case of a standard Minkowski metric $g^{\mu\nu} = \eta^{\mu\nu}$, these correspond to the homogeneous Dirichlet condition and Neumann conditions

$$ \partial_t \Phi|_B = 0, \quad \partial_i \Phi|_B = 0, $$

(6.95)
and the choice \( S = 0 \) corresponds to the Sommerfeld condition

\[
(\partial_t - \tilde{\partial}_t)\Phi|_{B} = 0. \tag{6.96}
\]

More generally, the geometric interpretation of these boundary conditions is obscured because the energy \( E \) (6.81) standardly used in the first-order theory is constructed with the linear space inner product, as opposed to the geometrically defined energy (6.16) natural to the second-order theory. It is possible to reformulate the covariant theory of the wave equation in first-order symmetric form with boundary conditions based upon the covariant energy (6.16). But without such a guide to begin with, a first-order symmetric hyperbolic formulation can lose touch with the underlying geometry.

This scalar-wave example also illustrates how the number of evolution variables and constraints escalates upon reduction to first-order form. As a result, in the case of Einstein’s equations, the advantages of utilizing symmetric hyperbolic theory are counterbalanced by the increased algebraic complexity which is further complicated by the wide freedom in carrying out a first-order reduction. See section 6.2.

6.3. The characteristic IBVP

There is another IBVP which gained prominence after Bondi’s [3] success in using null hypersurfaces as coordinates to describe gravitational waves. In the null-timelike IBVP, data are given on an initial characteristic hypersurface and on a timelike worldtube to produce a solution in the exterior of the worldtube. The underlying physical picture is that the worldtube data represent the outgoing gravitational radiation emanating from interior matter sources, while ingoing radiation incident on the system is represented by the initial null data.

The characteristic IBVP received little attention before its importance in general relativity was recognized. Rendall [57] established well-posedness of the double-null problem for the quasilinear wave equation, where data are given on a pair of intersecting characteristic hypersurfaces. He did not treat the characteristic problem head-on but reduced it to a standard Cauchy problem with data on a spacelike hypersurface passing through the intersection of the characteristic hypersurfaces so that well-posedness followed from the result for the Cauchy problem. He extended this approach to establish the well-posedness of the double-null formulation of the full Einstein gravitational problem. Rendall’s approach cannot be applied to the null-timelike problem, even though the double-null problem is a limiting case.

The well-posedness of the null-timelike problem for the gravitational case remains an outstanding problem. Only recently has it been shown that the quasilinear problem for scalar waves is well-posed [58]. The difficulty unique to this problem can be illustrated in terms of the one(spatial)-dimensional wave equation

\[
(\tilde{\partial}_t^2 - \tilde{\partial}_x^2)\Phi = 0, \tag{6.97}
\]

where \((\tilde{t}, \tilde{x})\) are standard spacetime coordinates. The conserved energy

\[
\tilde{E}(\tilde{t}) = \frac{1}{2} \int d\tilde{x}((\tilde{\partial}_t \Phi)^2 + (\tilde{\partial}_x \Phi)^2) \tag{6.98}
\]

leads to the well-posedness of the Cauchy problem. In characteristic coordinates \((t = \tilde{t} - \tilde{x}, x = \tilde{t} + \tilde{x})\), the wave equation transforms into

\[
\tilde{\partial}_t \partial_\tau \Phi = 0. \tag{6.99}
\]

The conserved energy evaluated on the characteristics \( t = \text{const} \),

\[
\tilde{E}(t) = \int dx(\partial_t \Phi)^2, \tag{6.100}
\]

no longer controls the derivative \( \partial_\tau \Phi \).
The usual technique for treating the IBVP is to split the problem into a Cauchy problem and local half-space problems and show that these individual problems are well-posed. This works for hyperbolic systems based upon a spacelike foliation, in which case signals propagate with finite velocity. For \((6.97)\), the solutions to the Cauchy problem with compact initial data on \(t = 0\) are square integrable and well-posedness can be established using the \(L^2\) energy norm \((6.98)\).

However, in characteristic coordinates, the one-dimensional wave equation \((6.99)\) admits signals traveling in the \(+x\)-direction with infinite coordinate velocity. In particular, initial data of compact support \(\Phi(0,x) = f(x)\) on the characteristic \(t = 0\) admit the solution \(\Phi = g(t) + f(x)\), provided that \(g(0) = 0\). Here \(g(t)\) represents the profile of a wave which travels from past null infinity \((x \to -\infty)\) to future null infinity \((x \to +\infty)\). Thus, without a boundary condition at past null infinity, there is no unique solution and the Cauchy problem is ill-posed. Even with the boundary condition \(\Phi(t, -\infty) = 0\), a source of compact support \(S(t,x)\) added to \((6.99)\), i.e.

\[
\partial_t \partial_x \Phi = S,
\]

produces waves propagating to \(x = +\infty\) so that although the solution is unique, it is still not square integrable.

On the other hand, consider the modified problem obtained by setting \(\Phi = e^{ax}\Psi\),

\[
\partial_t(\partial_x + a)\Psi = F, \quad \Psi(0,x) = e^{-ax}f(x), \quad \Psi(t, -\infty) = 0, \quad a > 0,
\]

\((6.102)\), where \(F = e^{-ax}S\). The solutions to \((6.102)\) vanish at \(x = +\infty\) and are square integrable. As a result, problem \((6.102)\) is well-posed with respect to an \(L^2\) norm. For the simple case where \(F = 0\), multiplication of \((6.102)\) by \((2a\Psi + \partial_x \Psi + \frac{1}{2} \partial_x^2 \Psi)\) and integration by parts gives

\[
\frac{1}{2} \partial_t \int dx ((\partial_x \Psi)^2 + 2a^2 \Psi^2) = \frac{a}{2} \int dx (2(\partial_x \Psi) \partial_x \Psi - (\partial_x \Psi)^2) \leq \frac{a}{2} \int dx (\partial_x \Psi)^2.
\]

The resulting inequality

\[
\partial_t E \leq \text{const} \ E
\]

for the energy

\[
E = \frac{1}{2} \int dx ((\partial_x \Psi)^2 + 2a^2 \Psi^2)
\]

\((6.104)\)

provides the estimates for \(\partial_t \Psi\) and \(\Psi\) which are necessary for well-posedness. Estimates for \(\partial_t \Psi\), and other higher derivatives, follow from applying this approach to the derivatives of \((6.102)\). The approach can be extended to include the source term \(F\) and other generic lower differential order terms. This allows well-posedness to be extended to the case of variable coefficients and, locally in time, to the quasilinear case.

Although well-posedness of the problem was established in the modified form \((6.102)\), the energy estimates can be translated back to the original problem \((6.101)\). The modification in going from \((6.101)\) to \((6.102)\) leads to an effective modification of the standard energy for the problem. Rewritten in terms of the original variable \(\Phi = e^{ax}\Psi\), \((6.105)\) corresponds to the energy

\[
E = \frac{1}{2} \int dx e^{-2ax}((\partial_x \Phi)^2 + a^2 \Phi^2).
\]

\((6.106)\)

Thus, while the Cauchy problem for \((6.101)\) is ill-posed with respect to the standard \(L^2\) norm, it is well-posed with respect to the exponentially weighted norm \((6.106)\).

This technique can be applied to a wide range of characteristic problems. In particular, it has been applied to the quasilinear wave equation for a scalar field \(\Phi\) in an asymptotically flat curved-space background with source \(S\),

\[
g^{\mu\nu} \partial_{\mu} \Phi = S(\Phi, \partial_x \Phi, x^\mu),
\]

\((6.107)\)
where the metric $g^{ab}$ and its associated covariant derivative $\nabla_a$ are explicitly prescribed functions of $(\Phi, x^a)$. In Bondi–Sachs coordinates \[3, 59\] based upon outgoing null hypersurface $u = \text{const}$, the metric has the form

$$
g_{\mu \nu} dx^\mu dx^\nu = -(e^{2\beta} W - r^{-2} h_{AB} W^A W^B) du^2 - 2 e^{2\beta} du dr - 2 h_{AB} W^B dx^A + r^2 h_{AB} dx^A dx^B,$$

(6.108)

where $x^A$ are angular coordinates, such that $(u, x^A) = \text{const}$ along the outgoing null rays, and $r$ is an areal radial coordinate. Here the metric coefficients $(W, \beta, W^A, h_{AB})$ depend smoothly upon $(\Phi, u, r, x^A)$ and fall off in the radial direction consistent with asymptotic flatness. The null-timelike problem consists in determining $\Phi$ in the exterior region given data on an initial null hypersurface and on an inner timelike worldtube,

$$
\Phi(0, r, x^A) = f(r, x^A), \quad \Phi(u, R, x^A) = q(u, x^A), \quad R \leq r < \infty, \quad u \geq 0.
$$

(6.109)

It is shown in \[58\] that

The null-timelike IBVP (6.107)–(6.109) is strongly well-posed subject to a positivity condition that the principal part of the wave operator reduces to an elliptic operator in the stationary case.

The proof is based upon energy estimates obtained in compactified characteristic coordinates extending to $I^+$.  

7. Historical developments

Early computational work in general relativity focused on the Cauchy problem. The IBVP only recently received serious attention and is still a work in progress. Although there are two formulations where strong well-posedness has been established (see sections 9 and 10), several important questions remain. Along the way, there have been partial successes based upon ideas of potential value in guiding future work.

7.1. The Frittelli–Reula formulation

The first extensive treatment of the IBVP for Einstein equations was carried out by Stewart \[15\], motivated at the time by the tremendous growth in computing power which made numerical relativity a realistic approach for applications to relativistic astrophysics. His primary goal was to investigate how to formulate an IBVP for Einstein’s equations which would allow unconstrained numerical evolution. Stewart focused upon a formulation of Einstein’s equations due to Frittelli and Reula \[60, 61\], although his approach is sufficiently general to have application to other formulations.

The Frittelli–Reula system was chosen because it is symmetric hyperbolic for certain choices of the free parameters. It is based upon the ADM formalism, with metric (2.13), in which all second derivatives are eliminated by the introduction of auxiliary variables. There is a two-parameter freedom in the choice of first-order variables. The densitized lapse $h^a\alpha$, where $p$ is an additional adjustable parameter, and the shift are treated as explicitly prescribed variables. In addition to the Hamiltonian and momentum constraints (2.10), the integrability conditions arising from the auxiliary variables lead to 18 additional constraints. Another adjustable parameter controls the freedom of mixing the constraints with the evolution system.

This net result is that the vacuum Einstein equations reduce to a first-order evolution system of the form (6.55) consisting of 30 equations governing the metric variables and 22 equations governing the constraints. This is further complicated by the lack of geometric or
tensorial properties of the evolution variables. Frittelli and Reula analyzed the principal part of the system and showed that it is symmetric hyperbolic for certain values of the adjustable parameters.

The well-posedness of the IBVP for such symmetric hyperbolic reductions of Einstein’s equations depends upon whether proper constraint-preserving boundary conditions can be imposed. Stewart analyzed the eigenvalues of the boundary matrix for the linearized system using the Fourier–Laplace method described in section 6.1.4. For the evolution system governing the metric variables, he identified six ingoing modes, six outgoing modes and eighteen zero-velocity modes in the kernel which propagate tangential to the boundary. Thus, this system requires exactly six boundary conditions. From the boundary matrix for the system governing constraint evolution, he identified three ingoing modes, three outgoing modes and sixteen zero-velocity modes, so that three boundary conditions are required for constraint enforcement.

The Fourier–Laplace analysis of the constraint system showed that the determinant condition (6.66) was satisfied, i.e. the homogeneous problem had only the trivial solution, and that the linearized system had a well-posed IBVP. The three boundary conditions could be satisfied by requiring that the Cauchy momentum constraints (2.17) vanish on the boundary.

The analysis of the evolution system governing the metric showed that the constraints could be enforced by a particular choice of boundary data for the metric variables. In this way, the evolution could be freed from the constraint system. The details are hidden in the symbolic algebra scripts necessary to analyze the complexity of the Fourier–Laplace modes. No discussion was given of the estimates for the derivatives which would be necessary for the well-posedness of the nonlinear problem. There has apparently been no further results for the Frittelli–Reula formulation and no attempt at a numerical evolution code.

Although the results were inconclusive for the nonlinear case, Stewart’s treatment provided the first example of how to apply pseudo-differential techniques to the IBVP for Einstein’s equations and served as the basis for much of the following work. The recognition that constraint preservation for this system could be achieved by enforcing the Cauchy momentum constraints on the boundary suggests a possible wider application but whether there is any universal procedure for enforcing the constraints in the $3+1$ formulation remains an open issue. See section 11 for a discussion.

7.2. The BSSN and NOR formulations

Codes based upon the Baumgarte–Shapiro–Shibata–Nakamura (BSSN) formulation [62, 63] have been used by the majority of groups [64–68] carrying out simulations of binary black hole and neutron star systems. The successful development of the BSSN formulation proceeded through an interplay between educated guesses and feedback from code performance. Only in hindsight has its success spurred mathematical analysis, which showed that certain versions were strongly hyperbolic and thus had a well-posed Cauchy problem [69–71]. Although significant progress has been made in establishing some of the necessary conditions for well-posedness and constraint preservation of the IBVP [72, 74, 75], there is still no satisfactory mathematical theory on which to base a numerical treatment of the boundary.

Similar to the Frittelli–Reula system, the BBSN system reduces the Einstein equations to first-order form by the introduction of auxiliary variables. In addition, there is a conformal-traceless decomposition of the 3-geometry. The Nagy–Ortiz–Reula (NOR) system [70] is similar but without the conformal decomposition. Again, a number of free parameters enter into the first-order reduction and into the way that the constraints are mixed with the evolution system. For a particular choice of parameters, the linearization off Minkowski
space is symmetric hyperbolic [75] and leads to a well-posed IBVP for the linearized problem. However, the corresponding nonlinear system is no longer symmetric hyperbolic and there is no well-posed boundary treatment.

Gundlach and Martin-Garcia [72] studied simplified second-order versions of the BSSN and NOR systems which were symmetric hyperbolic in a sense they defined in [73]. They were able to confirm and generalize many of the results found in [69] for the first-order reduction. Of particular interest, they found that all the characteristic modes propagated causally, in contrast to the superluminal modes present in the first-order system. The chief shortcoming of their treatment is the incompatibility of the constraints with the dissipative boundary conditions necessary for well-posedness.

The strong well-posedness of the IBVP for $3+1$ formulations remains an outstanding problem. The strategy in current numerical practice for BSSN evolution systems is to apply naive, homogeneous Sommerfeld boundary conditions, where needed, to each evolution variable (cf [68]) and place the boundary out far enough so that its harmful effects are limited.

7.3. Other $3+1$ studies

Many of the other early investigations on the well-posedness of the IBVP for $3+1$ formulations centered about linearized systems [77, 78, 83, 79], spherically symmetric and 1D spacetimes [84, 85, 87, 86] or other model problems [88–90, 73] which simplified the treatment. In particular, well-posedness of the linearized problem is a necessary condition for extension to the nonlinear case.

One promising approach was based upon a generalization of the Frittelli–Reula and Einstein–Christoffel (EC) [91] systems, which Kidder, Scheel and Teukolsky (KST) showed was symmetric hyperbolic for certain values of the free parameters [92]. In [78], energy estimates for maximally dissipative boundary conditions were used to formulate a well-posed IBVP for the linearization of this system off Minkowski space. However, constraint preservation limited the allowed boundary conditions to the reflecting Dirichlet or Neumann type.

The geometric analogy between the Hamiltonian and momentum constraints (2.10) of the Cauchy problem and the boundary constraints

$$G^{ab}N_b = 0, \tag{7.1}$$

where $N_b$ is the normal to the boundary, led Frittelli and Gomez to propose that (7.1) be enforced as boundary conditions [80–82]. They showed for the EC system, with vanishing shift and certain choices of the free parameters, that enforcing three linearly dependent combinations of the boundary constraints would lead to preservation of the Hamiltonian and momentum constraints. Furthermore, they showed that these linear combinations could be used to formulate boundary conditions for three of the ingoing metric variables. They did not study the boundary stability of the resulting IBVP.

In [83], the determinant condition (6.66) of the Fourier–Laplace method was applied to the linearized (EC) system to identify ill-posed modes arising from various choices of boundary conditions and free parameters. Several noteworthy results were found. For parameter choices in which the EC system was strongly but not symmetric hyperbolic, they found that maximally dissipative boundary conditions gave rise to ill-posed modes. This is in accord with the general theory which requires both maximally dissipative boundary conditions and a symmetric system to guarantee a well-posed IBVP. In addition, for a range of parameters giving rise to a symmetric system, ill-posed modes were found for boundary conditions based upon the

34
boundary constraints (7.1). As in the case of the Cauchy momentum constraints proposed by Stewart, this casts doubt on whether such boundary constraints are universally applicable. The approach in [83] was effective for ferreting out what does not work but did not go beyond the results of [78] for establishing a well-posed IBVP.

In a later study [93], the EC system was further generalized to include a dynamical lapse of the Bona–Masso type [94] and fixed shift. The IBVP was analyzed in the high-frequency limit, again using the determinant condition of the Fourier–Laplace method to determine ill-posed modes. It was found that constraint-preserving boundary conditions that were based upon the Newman–Penrose [95] Weyl curvature component \( \Psi_0 \) satisfied the determinant condition provided the evolution system was strongly hyperbolic and the constraint propagation system was symmetric hyperbolic. Boundary conditions based upon the Newman–Penrose \( \Psi_0 \) component were first introduced in the Friedrich–Nagy system [16]. Other \( \Psi_0 \) boundary conditions for the EC system were tested in [79, 89, 96–100, 102]. They have been improved to be highly effective absorbing boundary conditions for gravitational waves (see section 8) and have performed well in numerical tests. See section 13.

### 7.4. The harmonic and Z4 formulations

The IBVP for general relativity takes on one of its simplest forms in the harmonic formulation, in which the Einstein equations reduce to ten quasilinear wave equations. Nevertheless, progress on this problem was not straightforward. Difficulties arose in handling the harmonic constraints (2.2), in which derivatives of the metric tangential to the boundary prohibited use of standard dissipative boundary conditions for the wave equation. An early well-posed treatment was based upon the observation that the harmonic Cauchy problem is well-posed [13, 103]. Consequently, if locally smooth reflection symmetry were imposed across the boundary, then the well-posedness of the Cauchy problem would imply well-posedness of the resulting IBVP on either side of the boundary. The reflection symmetry not only forces the troublesome tangential derivatives to vanish but also forces homogeneous boundary conditions of the Dirichlet or Neumann type. Although these boundary conditions satisfy the dissipative criterion for a well-posed IBVP, they were too restrictive for use in practical numerical applications and did not allow large boundary data. It took a different approach to formulate a strongly well-posed harmonic IBVP with Sommerfeld-type boundary conditions. See section 10.

The Z4 formalism [104] aims at a covariant version of hyperbolic reduction by expressing the vacuum Einstein equations in the form

\[
G^\mu_\nu - \nabla^\mu Z^\nu + \frac{1}{2} g^{\mu\nu} \nabla_\eta Z^\eta = 0. \tag{7.2}
\]

When the vector field \( Z^\mu \) is identified with the (generalized) harmonic conditions \( C^\mu \), this reduces to the harmonic formulation. However, the freedom is retained to introduce other gauge conditions which force \( Z^\mu = 0 \). When only six components of (7.2) are required to vanish, it has been shown [105, 27] that the Z4 formalism encompasses the standard 3 + 1 formulations, including the ADM, NOR, BSSN and KST systems.

It is possible that the close analog between the Z4 and harmonic formulations might be used to shed light on the IBVP for 3 + 1 systems. Constraint-preserving boundary conditions for such Z4 systems have been proposed [106–108]. However, as for other 3 + 1 formulations, the boundary stability necessary for a strongly well-posed IBVP has not been established. Nevertheless, the results of numerical tests are promising. See section 13.
8. Non-reflecting outer boundary conditions

The correct physical description of an isolated system involves asymptotic conditions at infinity which ensure that the radiation fields have the proper $1/r$ falloff and that the total energy and radiative energy loss are finite. This can be achieved by locating the outer boundary at $I^+$. Instead, current simulations of binary black holes are carried out with an outer boundary at a large but finite distance in the wave zone, i.e. many wavelengths from the source. This is in accord with the standard practice in computational physics to impose an artificial boundary condition (ABC) which attempts to approximate the proper behavior of the exterior region.

At the analytic level, many ABCs are possible, even Dirichlet or Neumann conditions, provided the proper boundary data are known to allow outgoing radiation to pass through. However, the determination of the correct boundary data is a global problem, which requires extending the solution to $I^+$ either by matching to an exterior (linearized or nonlinear) solution obtained by some other means. The matching approach has been reviewed elsewhere [14]. As shown by Gustafsson and Kreiss, the construction of a non-reflecting boundary condition for an isolated system in general requires knowledge of the solution in a neighborhood of infinity [109].

Even if the outgoing-radiation data for the analytic problem were known, at the numerical level a Dirichlet or Neumann condition would reflect waves generated by the numerical error and trap them in the grid. The alternative approach is an ABC which is non-reflecting for homogeneous data. ABCs for an isolated radiating system for which homogeneous data are approximately valid are commonly called absorbing boundary conditions (see e.g. [110–116]), or non-reflecting boundary conditions (see e.g. [117–120]) or radiation boundary conditions (see e.g. [124, 125]). Such boundary conditions are advantageous for computational use. However, local ABCs are in general not perfect. Typically they cause some partial reflection of an outgoing wave back into the system [112, 116, 126, 127]. It is only required that there be no spurious reflection in the limit that the boundary approaches an infinite sphere.

A traditional ABC for the wave equation is the Sommerfeld condition. For a scalar field $\Phi$ satisfying the Minkowski space wave equation (6.1) with compact source, the exterior retarded field has the form

$$\Phi = \frac{f(t-r, \theta, \phi)}{r} + \frac{g(t-r, \theta, \phi)}{r^2} + \frac{h(t-r, \theta, \phi)}{r^3},$$

(8.1)

where $f$, $g$ and $h$ are smooth bounded functions. The simplest case is the monopole radiation field

$$\Phi = \frac{f(t-r)}{r},$$

(8.2)

which satisfies $(\partial_t + \partial_r)(r \Phi) = 0$. This motivates the use of the Sommerfeld condition

$$\frac{1}{r} (\partial_t + \partial_r) (r \Phi)|_R = q(t, R, \theta, \phi)$$

(8.3)

on a finite boundary $r = R$. However, a homogeneous Sommerfeld condition, i.e. $q = 0$, is exact only for the spherically symmetric monopole field. The Sommerfeld boundary data $q$ for the general case (8.1) falls off as $1/R^3$, so that a homogeneous Sommerfeld condition introduces an error which is small only for large $R$. As an example,

$$q = \frac{f(t-R) \cos \theta}{R^3}$$

(8.4)

for the dipole solution

$$\Phi_{\text{Dipole}} = \frac{\partial_t f(t-r)}{r} = -\left( \frac{f'(t-r)}{r} + \frac{f(t-r)}{r^2} \right) \cos \theta.$$  

(8.5)
A homogeneous Sommerfeld condition at \( r = R \) leads to a solution \( \tilde{\Phi}_{\text{Dipole}} \) containing a reflected ingoing wave. For large \( R \), it is given by

\[
\tilde{\Phi}_{\text{Dipole}} \sim \Phi_{\text{Dipole}} + \kappa \frac{F(t + r - 2R) \cos \theta}{r},
\]

where \( \partial_t f(t) = F(t) \) and the reflection coefficient has asymptotic behavior \( \kappa = O(1/R^2) \).

More precisely, the Fourier mode

\[
\tilde{\Phi}_{\text{Dipole}}(\omega) = \partial_z \left( \frac{e^{i\omega(t-r)}}{r} + \kappa \omega e^{i\omega(t+r-2R)/r} \right)
\]

satisfies the homogeneous boundary condition \((\partial_t + \partial_r) (r \tilde{\Phi}_{\text{Dipole}}(\omega))|_{R = 0} = 0\) with the reflection coefficient

\[
\kappa(\omega) = \frac{1}{2\omega^2 R^2 + 2i\omega R - 1} \sim \frac{1}{2\omega^2 R^2}.
\]

Use of this relationship simplifies the determination of the asymptotic falloff of the reflection coefficient by avoiding an explicit calculation of the reflected wave. Also note that if (8.3) is replaced by the second-order Sommerfeld condition

\[
\frac{1}{r^3} (\partial_t + \partial_r) r^2 (\partial_t + \partial_r) (r \Phi)|_{R = q_2} = 0,
\]

then dipole radiation has homogeneous data \( q_2 = 0 \). In this way, the falloff rate of the reflection coefficient is reduced from (8.8) to \( \kappa \sim 1/R^3 \).

The exponent \( n \) of the \( O(1/R^n) \) falloff of the reflection coefficient is an important measure of the accuracy of an ABC. Such reflection coefficients can be calculated for linearized gravitational waves on a Minkowski background, analogous to the above scalar-wave example, using either the Regge–Wheeler–Zerilli [128–130] perturbative method, as carried out in [99, 100, 102], or the Bergmann–Sachs [131] gravitational Hertz potential method, as carried out in [19]. See section 10.1. The main difference in the gravitational case arises from the gauge modes, which exist along with the radiative degrees of freedom. In first-order formulations, this is further complicated by the modes introduced by the auxiliary variables. The second-order harmonic formulation, in which all modes propagate on the light cone, is simplest to analyze. See section 10 for a discussion of reflection coefficients in the harmonic case.

Local ABCs have been extensively applied to linear problems with varying success [110, 112–115, 124, 126]. Some are local approximations to exact integral representations of the solution in the exterior of the computational domain [110], while others are based on approximating the dispersion relation of the so-called one-way wave equations [113, 126]. Higdon [112] showed that this last approach is essentially equivalent to specifying a finite number of angles of incidence for which the ABCs yield perfect transmission. Local ABCs have also been derived for the linear wave equation by considering the asymptotic behavior of outgoing wave solutions [124], thus generalizing the Sommerfeld condition. Although this type of ABC is relatively simple to implement and has a low computational cost, the final accuracy can be limited if the assumptions about the behavior of the waves are oversimplified. See [116, 118, 132, 133] for general discussions.

The disadvantages of local ABCs have led to the consideration of nonlocal versions based on integral representations of the infinite-domain problem [116, 118, 132, 133]. Even when the Green function was known, such approaches were initially dismissed as impractical [110]; however, the rapid development of computer power and numerical techniques has made it possible to implement exact nonlocal ABCs for the linear wave equation and Maxwell’s
equations in 3D [135, 136]. If properly implemented, this method can yield numerical solutions to a linear problem which converge to the exact infinite-domain problem in the continuum limit while keeping the artificial boundary at a fixed distance. However, due to nonlocality, the computational cost per time step usually grows at a higher power with grid size, $O(N^4)$ per time step in three spatial dimensions, than for a local approach [118, 132, 135].

The extension of ABCs to nonlinear problems is much more difficult. The problem is normally treated by linearizing the region between the outer boundary and infinity, using either local or nonlocal linear ABCs [133, 132]. The neglect of the nonlinear terms in this region introduces an unavoidable error at the analytic level. However, even larger errors are typically introduced in prescribing the outer boundary data. The correct boundary data must correspond to the continuity of fields and their normal derivatives when extended across the boundary into the linearized exterior. This is a subtle global requirement for any consistent boundary algorithm, since discontinuities in the field or its derivatives would otherwise act as a spurious sheet source on the boundary that would contaminate both the interior and the exterior solutions. However, the fields and their normal derivatives constitute an over determined set of data for the boundary problem. So it is necessary to solve a global linearized problem, not just an exterior one, in order to find the proper data. An expedient numerical method to eliminate back reflection is the use of sponge layers, cf [121], in which damping terms are introduced into the evolution equations near the outer boundary.

The designation 'exact ABC' is given to an ABC for a nonlinear system whose only error is due to linearization of the exterior. An exact ABC requires the use of global techniques, such as the boundary potential method, to eliminate back reflection at the boundary [120, 132]. Furthermore, nonlinear waves intrinsically backscatter, which makes it incorrect to try to entirely eliminate incoming radiation from the outer region. For the nonlinear wave equation, test results presented in [122, 123] showed that Cauchy-characteristic matching outperformed all ABCs in the existent literature.

It is an extra challenge to apply ABCs to strongly nonlinear hydrodynamic problems [118]. Thompson [137] generalized a previous nonlinear ABC of Hedstrom [117] to treat 1D and 2D problems in gas dynamics. These boundary conditions performed poorly in some situations because of difficulties in adequately modeling the field outside the computational domain [118, 137]. Hagstrom and Hariharan [138] have overcome these difficulties in 1D gas dynamics by their use of Riemann invariants. They proposed, at the heuristic level, a generalization of their local ABC to 3D.

In order to reduce the analytic error, an artificial boundary for a nonlinear problem must be placed sufficiently far from the strong-field region. This can increase the computational cost in multi-dimensional simulations [110]. There is no ABC which converges (as the discretization is refined) to the infinite-domain exact solution of a strongly nonlinear wave problem in multi-dimensions while keeping the artificial boundary fixed. When the system is nonlinear and not amenable to an exact solution, a finite outer boundary condition must necessarily introduce spurious effects. Attempts to use compactified Cauchy hypersurfaces which extend the domain to spatial infinity have failed because the phase of short-wavelength radiation varies rapidly in spatial directions [127]. In fact, in his pioneering simulation of binary black holes, Pretorius [28, 29] used this effect as a numerical expedience by applying artificial dissipation to diminish short-wavelength error arising from the use of a compactified outer boundary at spatial infinity. For a recent review of ABCs in the computational mathematics literature, see [139].

The situation for the gravitational IBVP is not as severe as for hydrodynamics, especially for formulations in which the gauge modes and radiation modes propagate with the same speed. However, due to nonlinearities, there is always some error of an analytic nature introduced by a finite boundary which is independent of discretization. In general, a systematic reduction of
this error can only be achieved by moving the computational boundary to larger and larger radii. There has been recent progress in designing absorbing boundary conditions for the gravitational field. Buchman and Sarbach \[99\] have developed higher order local boundary conditions based upon derivatives of \(\Psi_0\) which are non-reflecting up to any given multipole mode for linearized gravitational waves, analogous to the switch from a first-order Sommerfeld condition (8.3) to the second-order condition (8.10). These boundary conditions freeze the value of \(\Psi_0\) to its initial value, i.e.

\[
\dot{\Psi}_0 = 0,
\]

in order to avoid an \(O\)th-order violation of the compatibility condition between the initial and boundary data. They have extended this approach to include quadrupole gravitational waves on a Schwarzschild background and also to account for \(O(M/R)\) back scatter using a nonlocal version \[100\]. For a review of this approach, see [101]. It has been applied to the harmonic formulation in \[102\] and to the Z4 formulation in \[108\]. These are possibly the best possible local boundary conditions for the gravitational radiation modes.

Lau \[140–142\] has formulated an exact ABC for linearized gravitational waves on a Schwarzschild background. Based upon the flat-space work of \[120\], he reduces the calculation of the Green function incorporating the boundary condition for the perturbed metric to the integration of a radial ODE by using a combined spherical harmonic and Laplace transform of the Regge–Wheeler–Zerilli equations. He discusses the trade-off in computational cost for this nonlocal ABC versus the larger computational domain required by a local condition. This is similar to the trade-off between characteristic matching and the application of local boundary conditions.

9. The Friedrich–Nagy system

Friedrich and Nagy \[16\] have presented a theorem establishing the first strongly well-posed IBVP for Einstein’s equations with the generality to handle an outgoing-radiation boundary condition. The approach uses the energy method for first-order symmetric hyperbolic systems described in section 6.2.2. Their formulation is based upon the Einstein–Bianchi system of equations with evolution variables consisting of an orthonormal tetrad \(e_{\tilde{a}}, \tilde{a} = (0, 1, 2, 3)\), the associated connection coefficients \(\Gamma^a_{\tilde{a}b}\), and the Weyl curvature tetrad components \(C_{\tilde{a}b\tilde{c}\tilde{d}}\).

Although it differs from the metric-based formulations used in numerical relativity, the success of their treatment suggests that many of the underlying ideas should be universally applicable. In their words, ‘There are certainly many possibilities to discuss the initial boundary value problem and there will be as many ways of stating boundary conditions. However, all of these should be just modifications of the boundary conditions given in our theorem’. Perhaps this is overstated since their formulation is third differential order in the metric, as opposed to the second-order \(3 + 1\) or harmonic formulations. Yet, all successful formulations must have the common property of prescribing data which produces a unique solution to Einstein’s equations.

The tetrad vector \(e_0\) is chosen to be timelike and tangent to the boundary. It is used to construct the adapted coordinates \(x^a = (t, x^i) = (t, x, y, z)\) satisfying

\[
\mathcal{L}_{e_0} t = 1, \quad \mathcal{L}_{e_0} x^i = 0,
\]

so that \(e_0^\mu\) plays the role of the evolution vector field \(\tau^\mu\) introduced in section 4. However, the evolution field now has the metric property of being a timelike unit vector so, as a reminder, I denote it by \(T^\mu = e_0^\mu\). In accord with the notation in section 4, let the initial hypersurface \(S_0\) be given by \(t = 0\) and the boundary \(\mathcal{T}\) be given by \(x = 0\), with adapted coordinates \((t, x^i)\).
The tetrad vectors are adapted to the geometry as follows. Let \( N^\mu = e_1^\mu \propto -\nabla^\mu x \) be the unit outer normal to \( T \).

Extend \( N^\mu \) throughout the spacetime manifold \( M \) by requiring that it be the unit normal to the hypersurfaces \( T_c \) given by \( x = c = \text{const} > 0 \). On \( S_0 \), the remaining tetrad vectors \( e_A^\mu \), \( A = (2, 3) \), are chosen to be an orthonormal dyad for the \( (t = 0, x = c) \) subspaces. They are then propagated throughout \( M \) by Fermi–Walker transport along the integral curves of \( T^\mu \), which lie in \( T_c \). The connection components intrinsic to \( T_c \) are considered to be freely specifiable gauge source functions. In addition, the mean extrinsic curvature \( K \) of \( T_c \) is also considered to be a gauge source function. Moreover, it is shown that the equation \( K = q(x^\mu) \) can be cast as a quasilinear wave equation which determines \( T_c \) given initial data corresponding to \( x = c \) and \( \partial_t x = 0 \) at \( t = 0 \).

By design, this choice of adapted coordinates and tetrad gauge greatly simplify the IBVP. The evolution system consists of the gauge conditions governing the tetrad, the equations relating the connection to the tetrad, the vacuum equations relating the Weyl curvature to the connection (which imply the vanishing of the Einstein tensor) and the vacuum Bianchi identities, i.e. the tetrad version of the equations
\[
\nabla_\mu C_{\nu\rho\sigma}^\mu = 0. \tag{9.2}
\]
The system is over determined and subject to constraints arising from integrability conditions. Remarkably, it can be reduced to a system with the following properties.

- The evolution system is symmetric hyperbolic.
- The boundary matrix \( (6.76) \) admits two ingoing variables corresponding to combinations of the \( \Psi_0 \) and \( \Psi_4 \) Newman–Penrose components of the Weyl tensor.
- Maximally dissipative boundary conditions take the form
  \[
  \Psi_0 + \alpha \Psi_4 + \beta \bar{\Psi}_4 = q, \tag{9.3}
  \]
  where \( q \) is the (complex) boundary data and \( \alpha \) and \( \beta \) are coefficients subject to a dissipative condition. (Conventions here are chosen to be consistent with Newman–Penrose conventions and differ from \([16]\).)
- The subsidiary system governing the constraints is symmetric hyperbolic and intrinsic to the \( T_c \) hypersurfaces, i.e. all derivatives are tangential to \( T_c \). This gives rise to constraint preservation without requiring any further restrictions on the boundary conditions.

The resulting IBVP is strongly well-posed. Given initial data on \( S \), including the hyperbolic angle \( \Theta \) in \( (3.4) \) at the edge \( B_0 \), the boundary data \( q \), a choice of gauge source functions and a dissipative choice of boundary condition, there exists a unique solution locally in time. Furthermore, the solution depends continuously on the data.

Several important points should be noted.

- The specification of the mean extrinsic curvature \( K \) of the boundary geometrically determines the location of the boundary.
- The choice of unit timelike vector \( T^t \) tangent to the boundary represents gauge freedom in the construction of the solution. It induces a corresponding foliation of the spacetime and the boundary according to \( L_{T^t} t = 1 \).
- The geodesic curvature of the integral curves of \( T^\mu \) constitutes gauge source functions required on the boundary. This gauge freedom feeds into the adapted coordinates \( (t, x^A) \) of the boundary. As a result, the functional specification of \( K(t, x^A) \) becomes gauge dependent. This complication could be avoided by choosing \( T^\mu \) to be geodesic but at the expense of possible coordinate focusing singularities which would affect the long-term existence of the solution.
10. The harmonic IBVP

The first successful treatment of the harmonic IBVP for Einstein’s equations was carried out using the pseudo-differential theory described in section 6.1.4, which established strong well-posedness in a generalized sense [17]. The theory was developed for the second-order formulation of the generalized harmonic formulation (2.2)–(2.5). The boundary conditions were given in Sommerfeld form in terms of the outgoing null vector \( K^a = T^a + N^a \) normal to the foliation of the boundary. Here, as in the Friedrich–Nagy approach (9.4), \( T^a \) is a future-directed timelike unit vector tangent to the boundary but now it is also chosen to be normal to its foliation \( \mathcal{B}_s \). Recall that \( n^a \), the normal to the Cauchy foliation \( \mathcal{S}_s \), is not necessarily tangent to the boundary. The motion of the boundary, characterized by the hyperbolic angle (3.4), distinguishes \( T^a \) from \( n^a \).

In the adapted coordinates \( x^\mu = (t \geq 0, x^i \geq 0, \chi \) described in (4.3), six Sommerfeld boundary conditions for the densitized metric \( \gamma^{\mu\nu} = \sqrt{-g}\hat{g}^{\mu\nu} \) were given by

\[
\begin{align*}
K^\mu \partial_\mu \gamma^{AB} &= q^{AB}(t, x^i) \\
K^\mu \partial_\mu (\gamma^{tA} + \gamma^{tA}) &= q^t(t, x^i) \\
K^\mu \partial_\mu (\gamma^{tt} + 2\gamma^{tx} + \gamma^{xx}) &= q(t, x^i),
\end{align*}
\]

where the \( q^s \) are freely prescribed Sommerfeld data. The harmonic constraints (2.2) were used to supply four additional boundary conditions, which could be expressed in the Sommerfeld form

\[
\begin{align*}
\sqrt{-g}G^A &= \frac{1}{2}(\partial_i - \partial_\chi)(\gamma^{tA} - \gamma^{tA}) + \frac{1}{2}(\partial_i + \partial_\chi)(\gamma^{tA} + \gamma^{tA}) + \partial_\mu \gamma^{AB} - \sqrt{-g}\hat{g}^A = 0 \\
\sqrt{-g}(C' + C^t) &= \frac{1}{2}(\partial_i - \partial_\chi)(\gamma^{tt} - \gamma^{tt}) + \frac{1}{2}(\partial_i + \partial_\chi)(\gamma^{tt} + 2\gamma^{tx} + \gamma^{xx}) \\
&\quad + \partial_\chi (\gamma^{tA} + \gamma^{tA}) - \sqrt{-g}(\hat{g}' + \hat{g}^t) = 0 \\
\sqrt{-g}C^i &= \frac{1}{2}(\partial_i - \partial_\chi)(\gamma^{tt} - \gamma^{tt}) + \frac{1}{2}(\partial_i + \partial_\chi)(\gamma^{tt} - \gamma^{tt}) \\
&\quad \times (\gamma^{tt} + 2\gamma^{tx} + \gamma^{xx}) + \partial_\chi y^{tA} - \sqrt{-g}\hat{g}' = 0.
\end{align*}
\]

Constraint preservation then follows from the homogeneous wave equation (2.6).

The key feature of (10.1)–(10.6) is that they form a sequential hierarchy of Sommerfeld boundary conditions for the metric variables such that the source terms are given in terms of derivatives of previous variables in the sequence. For instance, the terms on the second line of (10.4) are derivatives of \( \gamma^{AB} \) and \( \gamma^{tA} + \gamma^{tA} \), whose boundary conditions are prescribed previously in (10.1) and (10.2). This pattern persists for the remaining boundary conditions in the sequence, i.e. (10.5) and (10.6). This structure gives rise to a corresponding sequence of estimates for the variables in the hierarchy, which is the key for establishing boundary stability and the strong well-posedness of the IBVP. There is considerable freedom in the boundary conditions provided this hierarchical structure is preserved.
The well-posedness of the harmonic IBVP was subsequently also established using estimates for the non-standard energy (6.16) associated with a timelike vector pointing outward from the boundary [18]. The hierarchical structure of the boundary conditions corresponds to the upper triangular property (6.1.3), which is a sufficient condition for a well-posed IBVP for a coupled system of quasilinear wave equations.

A more general and geometrical version of these results in terms of a background metric $\tilde{g}_{ab}$ was presented in [19]. The connection $\nabla$ and curvature tensor $\tilde{R}^c_{\ abc}$ associated with the background metric $\tilde{g}_{ab}$ have the same tensorial properties as the corresponding quantities $\nabla_a$ and $R^c_{\ abc}$ associated with $g_{ab}$. In particular, the difference $\nabla_a - \nabla_a$ defines a tensor field $C^d_{\ ab}$ according to

\[
(\nabla_a - \nabla_a^\dag) v^d = C^d_{\ ab} v^b
\]

for any vector field $v^b$. In terms of the (nonlinear) perturbation $f_{ab} = g_{ab} - \tilde{g}_{ab}$ (10.8)
of the metric from the background,

\[
C^d_{\ ab} = \frac{1}{2} g^{de} \left( \tilde{\nabla}_a f_{bc} + \tilde{\nabla}_a f_{bc} - \nabla_c f_{ab} \right).\]

(10.9)

Since $\tilde{g}_{ab}$ is explicitly known, a solution for $f_{ab}$ is equivalent to a solution for $g_{ab}$. Einstein’s equations are given by

\[
E^{ab} := G^{ab} - \nabla^a (\nabla^b \tilde{f}_{cd}) + \frac{1}{2} g^{de} \nabla_d C^e_{\ ab} = 0
\]

subject to the harmonic constraints

\[
\hat{C}^\rho := g^{\rho \nu} (\Gamma^\rho_{\ \mu \nu} - \nabla^\rho \tilde{g}_{\ \mu \nu}) = 0.
\]

(10.12)

In the adapted coordinates, the harmonic constraints take the form

\[
\hat{C}^\rho := g^{\rho \nu} (\Gamma^\rho_{\ \mu \nu} - \nabla^\rho \tilde{g}_{\ \mu \nu}) = 0.
\]

(10.12)

so that the background Christoffel symbols $\Gamma^\rho_{\ \mu \nu}$ appear as harmonic gauge source functions. When the harmonic constraints are satisfied, the reduced Einstein equations form the desired quasilinear wave system for $f_{\ \mu \nu}$,

\[
g^{\rho \nu} \nabla_\rho f_{\mu \nu} &= 2 g_{\alpha \delta} g^{\eta \sigma} C_\alpha^{\ \mu \nu} C_\sigma^{\ \eta \epsilon} + 4 c^B_{\ \sigma (\mu} g_{\nu \lambda)} C_\sigma^{\ \eta \epsilon} g^{\sigma \tau} - 2 g^{\rho \sigma} \tilde{R}^\rho_{\ \rho \sigma (\mu} g_{\nu \lambda)}.
\]

(10.13)

The analogs of the Sommerfeld conditions (10.1)–(10.6) are prescribed in terms of the boundary decomposition of the metric

\[
g_{ab} = N_a N_b + H_{ab}, \quad H_{ab} = - T_a T_b + Q_{ab}.
\]

(10.14)

This leads to an orthonormal tetrad $(T^a, N^a, Q^a, \bar{Q}^a)$ on $\mathcal{T}$, where $Q^a$ is a complex null vector tangent to $\mathcal{E}_t$ with normalization

\[
Q_{ab} = Q_{a(\bar{Q}b)}, \quad Q^a \bar{Q}_a = 2, \quad Q^a Q_a = 0.
\]

(10.15)

(The tetrad is unique up to the spin freedom $Q^a \rightarrow e^{\alpha a} Q^\alpha$ which does not enter in any essential way.) In terms of the outgoing and ingoing null vector fields $K^a = T^a + N^a$ and $L^a = T^a - N^a$, respectively, which are normal to $\mathcal{E}_t$, the metric has the null tetrad decomposition

\[
g_{ab} = - K_a L_b + Q_{a(\bar{Q}b)}.
\]

(10.16)

Six Sommerfeld boundary conditions which determine the components of the outgoing null derivatives $K^a \nabla_a f_{bc}$ are then given by

\[
\frac{1}{2} K^a K^b K^c \nabla_a f_{bc} = q^a K_a,
\]

(10.17)
\[(Q^b K^c K^a - \frac{1}{2} K^b K^c Q^a) \nabla_a f_{bc} = q^a Q_a, \]  
\[(L^b K^c K^a - \frac{1}{2} K^b K^c L^a) \nabla_a f_{bc} = q^a L_a, \]  
\[(\frac{1}{2} Q^b Q^c K^a - Q^b K^c Q_a) \nabla_a f_{bc} = 2\sigma, \]

in terms of the boundary data \(q^a\) and \(\sigma\). The harmonic constraints provide four additional boundary conditions which, in terms of the null tetrad, can be expressed in the Sommerfeld form

\[-2C_a K_a = (Q^b \bar{Q}^c K^a + K^b K^c \bar{L}^a - K^b \bar{Q}^c Q^a - K^b Q^c \bar{Q}^a) \nabla_a f_{bc} = 0, \]  
\[-2C_a Q_a = (L^b Q^c K^a + K^b Q^c \bar{L}^a - K^b L^c Q^a + Q^b \bar{Q}^c \bar{Q}^a) \nabla_a f_{bc} = 0, \]  
\[-2C_a L_a = (L^b L^c K^a + Q^b \bar{Q}^c L^a - \bar{Q}^b \bar{L}^c Q^a - \bar{Q}^b \bar{Q}^c \bar{L}^a) \nabla_a f_{bc} = 0. \]

As before, constraint preservation follows from (2.6).

Together, (10.17)–(10.23) provide Sommerfeld boundary conditions for the components of \(K^a \nabla_a f_{bc}\) in the sequential order \((KK), (QK), (LK), (QQ), (Q\bar{Q}), (LQ), (LL))\) in terms of the boundary data and the derivatives of preceding components in the sequence. This hierarchy of Sommerfeld boundary conditions satisfies the requirements given in section 6.1.3 (theorem 1 of [19]) for a strongly well-posed IBVP for the quasilinear hyperbolic system (10.13). See section 12 for a geometrical interpretation of the boundary data and section 13 for numerical tests.

10.1. Application to an isolated system

The main application of the gravitational IBVP is to the spherical outer boundary used in the simulation of an isolated system emitting radiation. As discussed in section 8, in the absence of an exterior solution, the simplest approach is the use of a Sommerfeld boundary condition with homogeneous data. In doing so, it is important to take advantage of the freedom in the form of the boundary conditions in order to reduce back reflection.

Sommerfeld boundary conditions consistent with a well-posed harmonic IBVP have wide freedom regarding the addition of (i) partial derivative terms consistent with the hierarchical structure and (ii) lower order algebraic terms. Various choices were considered in [19]. They were tested by computing the resulting reflection coefficients for spherical waves in a Minkowski space background. For this purpose, the densitized metric is approximated to linearized accuracy by

\[\sqrt{-\eta^{\mu\nu}} = \eta^{\mu\nu} + \gamma^{\mu\nu},\]

where \(\eta^{\mu\nu}\) is the Minkowski metric. The calculation of the reflection coefficients proceeds as for the scalar-wave example in section 8, as modified to deal with the gauge modes.

Linearized waves in the harmonic gauge can be constructed from the gravitational analog of the Hertz potential [131], which has the symmetries

\[H^{\mu\nu\alpha\beta} = H^{\alpha\nu\beta\mu} = H^{\nu\alpha\beta\mu} = H^{\nu\beta\mu\alpha}\]

and satisfies the flat-space wave equation \(\partial^\sigma \partial_\sigma H^{\mu\nu\alpha\beta} = 0\). Then the perturbation \(\gamma^{\mu\nu} = \partial_\alpha \partial_\beta H^{\mu\nu\alpha\beta}\) satisfies the linearized Einstein equations \(\partial^\sigma \partial_\sigma \gamma^{\mu\nu} = 0\) in the harmonic gauge \(\partial_\nu \gamma^{\mu\nu} = 0\).

Outgoing waves can be generated from the potential

\[H^{\mu\nu\alpha\beta} = K^{\mu\nu\alpha\beta} \frac{f(t - r)}{r}, \quad \gamma^{\mu\nu} = K^{\mu\nu\alpha\beta} \partial_\alpha \partial_\beta \frac{f(t - r)}{r},\]

where \(f(t - r)\) is the incoming wave function. The calculation of the reflection coefficients proceeds as for the scalar-wave example in section 8, as modified to deal with the gauge modes.
where \( K^{\mu\nu\alpha\beta} \) is a constant tensor. (All higher multipoles can be constructed by taking spatial derivatives.) \( K^{\mu\nu\alpha\beta} \) has 21 independent components but the choice \( K^{\mu\nu\alpha\beta} = \epsilon^{\mu\nu\alpha\beta} \) leads to \( \gamma^{\mu\nu} = 0 \), so there are only 20 independent waves. These can be reduced to ten pure gauge waves for which the linearized Riemann tensor vanishes, which correspond to the trace terms in \( K^{\mu\nu\alpha\beta} \); e.g. \( K^{\mu\nu\alpha\beta} = \eta^{\alpha\mu} \eta^{\beta\nu} - \eta^{\mu\nu} \eta^{\alpha\beta} \) leads to a monopole gauge wave. The trace-free part gives rise to ten independent quadrupole gravitational waves, corresponding to spherical harmonics with \( (\ell = 2, -2 \leq m \leq 2) \) in the two independent polarization states.

For a boundary at \( r = R \), the Sommerfeld derivative in the outgoing null direction is

\[
K^\mu \partial_\mu = \partial_t + \frac{1}{r} \partial_r.
\]

In formulating boundary conditions which minimize back reflection, the property \( K^\mu \partial_\mu f(t - r) = 0 \) is used to introduce the appropriate powers of \( r \), analogous to the scalar example (8.3).

In [19], the optimal choice was found to be the Sommerfeld hierarchy

\[
\begin{align*}
\frac{1}{r^2} K_\alpha K_\beta K^\mu \partial_\mu (r^2 \gamma^{\alpha\beta}) &= q_{KK}, \\
\frac{1}{r^2} K_\alpha Q_\beta K^\mu \partial_\mu (r^2 \gamma^{\alpha\beta}) &= q_{KQ}, \\
\frac{1}{r} Q_\alpha Q_\beta K^\mu \partial_\mu (r^2 \gamma^{\alpha\beta}) - \frac{\gamma}{r} &= q_{QQ}.
\end{align*}
\]

It was found that the data \( q_\ldots = O(1/R^4) \) for the outgoing gravitational quadrupole waves and \( q_\ldots = O(1/R^3) \) for the outgoing gauge waves. This implies, in accord with (8.9), that homogeneous Sommerfeld data give rise to the reflection coefficients \( \kappa = O(1/R^3) \) for the gravitational waves and \( \kappa = O(1/R^2) \) for the gauge waves. These results were confirmed using the Regge–Wheeler–Zerilli perturbative formulation along with the metric reconstruction method described in [130].

The analysis of linearized waves shows that \( q_{QQ} \) controls the amplitude of the gravitational radiation passing through the boundary. Higher order boundary conditions can be based upon replacing (10.30) by a condition on \( \Psi_0 \), which in the linearized theory controls the radiation in a gauge-independent manner. In this way, the \( \Psi_0 \)-based boundary conditions discussed in section 8 can be used to further increase the \( 1/R^n \) falloff rate of the reflection coefficients for gravitational waves.

11. Constraint preservation

The IBVP for Einstein’s equations is still not well understood due to a great extent from complications arising from the constraints. The Hamiltonian and momentum constraints on the Cauchy data take the universal form (2.10) in terms of the components of the Einstein tensor normal to the initial hypersurface. However, there is no common way to ensure constraint preservation for the various formulations of Einstein’s equations. Even the constraints themselves take on different forms.

The Friedrich–Nagy system (see section 9) is based upon the Einstein–Bianchi equations which are third differential order in terms of the metric. In that case, by a cleverly designed choice of adapted coordinates and gauge, constraint propagation is governed by a system tangential to the boundary. Thus, there are no ingoing constraint modes and constraint preservation is straightforward.

In the strongly well-posed harmonic system described in section 10, the harmonic conditions \( C^\alpha \) became surrogates for the Hamiltonian and momentum constraints. Because
Cμ satisfies a homogeneous wave equation, there are four ingoing constraint modes. These could be eliminated by dissipative boundary conditions with homogeneous data. In section 10, homogeneous Dirichlet conditions on Cμ were chosen. This allowed the constraints to be enforced in terms of first differential Sommerfeld conditions on the metric. Homogeneous Neumann or Sommerfeld conditions on the constraints would also ensure constraint preservation but at the expense of a more complicated coupling with the evolution system for the metric.

The worldtube constraints which arise in the gravitational version of the null-timelike IBVP discussed in section 6.3 present an entirely different aspect. In that problem, boundary data on a worldtube T and initial data on an outgoing null hypersurface N0 determine the exterior spacetime by integration along the outgoing null geodesics. The worldtube constraints impose conditions on the integration constants. The Bondi–Sachs formalism [3, 59] introduces the coordinates xμ = (u, r, xA) based upon a family of outgoing null hypersurfaces Nu, where u labels the null hypersurfaces, xA are angular labels for the null rays and r is a surface area coordinate. The evolution system is composed of radial propagation equations along the outgoing null rays consisting of the hypersurface equations Gμν = Gνμ = 0, which only contain derivatives tangent to Nu, and the evolution equations G_AB = 1/2 g^CD G CD = 0.

The components of Einstein’s equations independent of the hypersurface and evolution equations are worldtube constraints (called supplementary conditions by Bondi and Sachs),

\[ g^{AB}G_{AB} = 0 \]  \hspace{1cm} (11.1)
\[ G'_{\mu} = 0 \]  \hspace{1cm} (11.2)
\[ G''_{\mu} = 0. \]  \hspace{1cm} (11.3)

When the hypersurface and evolution equations are satisfied, the contracted Bianchi identity

\[ \nabla_\nu G'_{\nu} = 0 \]  \hspace{1cm} (11.4)
implies that these equations need only be satisfied on the worldtube T. The identity for \( \mu = r \) reduces to \( g^{AB}G_{AB} = 0 \) so that (11.1) becomes trivially satisfied. (Here it is necessary that the worldtube have non-vanishing expansion so that the areal radius r is a non-singular coordinate.)

The identity for \( \nu = A \) then reduces to the radial ODE

\[ \partial_r (r^2 G'_{\mu}) = 0, \]  \hspace{1cm} (11.5)
so that \( G'_{A} \) vanishes if it vanishes on T. When \( G'_{A} = 0 \), the identity for \( \nu = u \) then reduces to

\[ \partial_u (r^2 G''_{\mu}) = 0, \]  \hspace{1cm} (11.6)
so that \( G''_{\mu} \) also vanishes if it vanishes on T.

Thus, the worldtube constraints reduce to (11.2) and (11.3), which are equivalent to the condition that the Einstein tensor satisfies

\[ \xi^\mu G'_{\mu}N_r = 0, \]  \hspace{1cm} (11.7)
where \( \xi^\mu \) is any vector field tangent to the worldtube, whose normal is \( N_r \). These are the boundary analog of the momentum constraints for the Cauchy problem. In Stewart’s treatment of the 3 + 1 IBVP (see section 7.1), it was the Cauchy momentum constraints which were enforced on the boundary. In the characteristic IBVP, it is the worldtube constraints (11.7) which must be enforced. They form three components of the boundary constraints (7.1) proposed by Frittelli and Gomez for the 3 + 1 problem. (See section 7.3.)

This worldtube constraints (11.7) can be interpreted as flux conservation laws for the \( \xi \)-momentum contained in the worldtube [143],

\[ P_\xi (u_2) - P_\xi (u_1) = \int_{u_1}^{u_2} dS_u \{ \nabla^\nu \nabla_\mu \xi^\mu - \nabla_\mu \nabla^{(\nu)\xi^\mu} \}, \]  \hspace{1cm} (11.8)
where

\[ P_\xi = \oint dS_{\mu \nu} \nabla^\nu [\xi^\mu] \]  

(11.9)

and \(dS_{\mu \nu}\) and \(dS_\nu\) are the 2-surface and 3-volume elements on the worldtube. When \(\xi^\mu\) is a Killing vector for the intrinsic 3-metric of the worldtube, this gives rise to a strict conservation law. For the limiting case at \(I^+\), these flux conservation laws govern the energy–momentum, angular momentum and supermomentum corresponding to the asymptotic symmetries [143]. For an asymptotic time translation, they give rise to the Bondi’s famous result [3] relating the mass loss to the square of the news function.

In terms of the intrinsic metric of the worldtube

\[ H_{\mu \nu} = g_{\mu \nu} - N_\mu N_\nu, \]

(11.10)

its intrinsic covariant derivative \(D_\mu\) and its extrinsic curvature

\[ K_{\mu \nu} = H_\mu ^\rho \nabla_\rho N_\nu, \]

(11.11)

the worldtube constraints (11.7) can be rewritten as

\[ H_\mu ^\delta G_{\mu \rho} N_\rho = D_\mu (K_\rho ^\delta - \delta_\rho \delta_\mu K_\rho ^\rho) = 0. \]

(11.12)

These are the analog of (2.17) for the Cauchy problem but they now form a symmetric hyperbolic system because of the timelike nature of the worldtube. In terms of a dyad (10.15) adapted to the foliation of the worldtube, this gives rise to the

**Worldtube theorem** [144]. Given \(H_{ab}, Q^a Q^b K_{ab}\) and \(K\), the worldtube constraints constitute a well-posed initial-value problem which determines the remaining components of the extrinsic curvature \(K_{ab}\).

The theorem constrains the integration constants for the nullcone-worldtube IBVP. Similarly, they constrain the boundary data for a 3 + 1 IBVP subject to the Frittelli–Gomez conditions. Unfortunately, for neither of these IBVPs has it been possible to combine the boundary constraints with the evolution system in a manner consistent with a strongly well-posed IBVP.

The enforcement of the boundary constraints is an indirect way to enforce the Hamiltonian and momentum constraints \(H = G^{\alpha \nu} n_\alpha n_\nu\) and \(P^\alpha = h^{\alpha \nu} G^{\nu \sigma} n_\sigma\), where in the 3 + 1 decomposition with respect to the Cauchy hypersurfaces,

\[ h_{\mu \nu} = g_{\mu \nu} + n_\mu n_\nu. \]

The more direct approach commonly used to investigate constraint preservation in the 3 + 1 Cauchy problem is to cast the contracted Bianchi identity (11.4) into a hyperbolic system. The results depend upon the particular formulation.

As a first example, consider the ADM system (2.15) in which only the six Einstein equations

\[ h^{\nu \rho} h^{\rho \sigma} R_\sigma ^\nu = 0 \]

(11.13)

are evolved. Application of the contracted Bianchi identity gives rise to the symmetric hyperbolic constraint propagation system

\[ n^\nu \partial_\nu H - \partial_\mu P^\mu = B^\nu G_{\nu \gamma} n^\gamma \]

\[ n^\nu \partial_\nu P^\mu - h^{\gamma \mu} \partial_\nu H = B^{\nu \gamma} G_{\nu \gamma} n^\nu, \]

(11.14)

where the coefficients \(B^\nu\) and \(B^{\nu \gamma}\) arise from Christoffel symbols and do not enter the principal part. When applied to the IBVP, a complication arises from the component of the shift normal to the boundary,

\[ \beta^\mu = \beta^\mu N_\mu = -\alpha \sinh \Theta \]

(11.15)
in terms of the lapse \( \alpha \) and the hyperbolic angle \( \Theta \) (3.4) governing the velocity of the boundary. Here \( \beta^N < 0 \) (\( \beta^N > 0 \)) for a boundary which is moving inward (outward) with respect to the Cauchy hypersurfaces. An analysis of (11.14) shows that only one boundary condition is allowed provided \( \beta^N \leq 0 \), i.e. provided the boundary is moving inward. In that case, the theory of symmetric hyperbolic systems guarantees that all the constraints would be preserved if the single constraint

\[
H + \frac{\partial}{\partial \tau} \mathcal{N} = G_{\mu\nu} n^\mu K^\nu = 0
\]  

is satisfied at the boundary, where \( K^\mu \) is the outgoing null vector to the foliation of the boundary. (Additional boundary conditions are necessary for constraint preservation if \( \beta^N > 0 \).) By virtue of the evolution system (11.13), constraint (11.16) is equivalent to

\[
G_{\mu\nu} K^\mu K^\nu = 0.
\]

This is the Raychaudhuri equation (cf [145])

\[
K^\mu \partial_\mu \theta + \frac{1}{2} \theta^2 + \sigma \bar{\sigma} = 0,
\]

where \( \theta \) is the expansion and \( \sigma \) is the shear of the outgoing null rays tangent to \( K^\mu \). Thus, for the ADM system, constraint preservation can be enforced by the Sommerfeld boundary condition (11.18) for \( \theta \). Unfortunately, although the constraint system has these attractive properties, the ADM evolution system is only weakly hyperbolic and consequently leads to unstable evolution.

Next consider the BSSN evolution system, which enforces the six Einstein equations

\[
h_{\mu}^\rho h_{\nu}^\sigma R_{\rho\sigma} - \frac{2}{3} h_{\mu}^\nu H = 0.
\]

The contracted Bianchi identity now implies the constraint system

\[
n^\gamma \partial_\gamma H - \partial_j P^j = B^\gamma G_{\nu\gamma} n^\nu
\]

\[
n^\gamma \partial_\gamma P^j + \frac{1}{2} h^{ij} \partial_j H = B^{\nu\gamma} G_{\nu\gamma} n^\nu.
\]

This is not symmetric hyperbolic and would not lead to stable constraint preservation even for the Cauchy problem. This is remedied in the course of introducing auxiliary variables which reduce the BSSN system to first-order form. Auxiliary constraints are mixed into the evolution system (11.19) and they combine with the constraint system (11.21) to form a larger symmetric hyperbolic constraint system. There is a large freedom in the constraint-mixing parameters and gauge conditions. For a particular choice made by Núñez and Sarbach [75], the linearization off Minkowski space yields a symmetric hyperbolic evolution system. The boundary conditions for this system are complicated by the normal component of the shift. As discussed in conjunction with (3.5), the number of boundary conditions required by the advection equations introduced in the first-order reduction depends upon whether \( \beta^N \) is positive or negative. This forces use of a Dirichlet condition, e.g. \( \beta^N = 0 \), rather than a Sommerfeld condition on the shift. Constraint preservation holds only in a certain parameter range, \( (b_1 \leq 1, b_2 \leq 1) \) for the boundary conditions given in equation (97) of [75]. The particular choice \( b_1 = 0 \) leads to the boundary condition [146]

\[
H - 3P^\mu \mathcal{N}_\mu = G_{\mu\nu} n^\mu (n^\nu - 3N^\nu) = \mathcal{Z}, \]

where \( \mathcal{Z} \) represents contributions from the auxiliary constraints, or, by using the evolution system (11.19),

\[
G_{\mu\nu} L^\mu L^\nu = \mathcal{Z},
\]
where \( L^\mu \) is the ingoing null vector to the boundary. It is a bizarre feature of the \( 3+1 \) problem that the constraint-preserving boundary condition switches from the outgoing Raychaudhuri form (11.17) to the ingoing Raychaudhuri form (11.23) in going from the ADM to the BSSN system. The Raychaudhuri equation for the outgoing null direction cannot be imposed in the allowed range of \((b_1, b_2)\).

The widely varying nature of constraint enforcement among different formulations does not provide any apparent insight. However, one problem common to many first-order formulations arises from the advective derivative \( n^\mu \partial_\mu \), which determines whether the auxiliary variables are ingoing or outgoing at the boundary, depending on the sign of \( \beta^N \). This problem could be avoided by instead using the derivative \( t^\mu \partial_\mu \), determined by the evolution field, which can always be chosen tangential to the boundary. This suggests that the projection operator \( \pi^\mu_\nu \) associated with \( t^\mu \), given in (4.4), might be useful in separating out the evolution system from the constraints, rather than the projection operator \( h^\mu_\nu \) used in (11.13) and (11.19). This gives rise to many ways to obtain a symmetric hyperbolic constraint system whose boundary treatment is independent of \( \beta^N \). As a simple example, in adapted coordinates the evolution system \( G^{ij} = \lambda \delta^{ij} G_{tt} \), with \( \lambda > 0 \), leads via (11.4) to the symmetrizable constraint system

\[
\partial_t G^{tt} + \partial_j G^{jt} = \text{lower order terms}
\]
\[
\partial_t G^{ti} + \lambda \partial_t G^{tt} = \text{lower order terms.} \quad (11.24)
\]

Independently of \( \beta^N \), this system requires only one boundary condition to preserve all the constraints.

12. Geometric uniqueness of the IBVP

The solution of the Cauchy problem has the important property of geometric uniqueness, i.e. Cauchy data \((h_{ab}, k_{ab})\) on \( S_0 \) determine a metric \( g_{ab} \) which is unique up to diffeomorphism. Under a diffeomorphism \( \psi \), the data \((\psi^* h_{ab}, \psi^* k_{ab})\) determine an equivalent metric. As well as being a pretty result, this has the practical application of allowing numerical simulations with the same initial data but carried out with different formulations and different gauge conditions to produce geometrically equivalent spacetimes. Friedrich [35] has emphasized that this property remains an unresolved issue for the IBVP.

There are different ways in which this property might be formulated for the IBVP. The most demanding way would be to require that the data at a point of the boundary be locally determined by the boundary geometry in the neighborhood of that point. Such data might include the trace \( K \) of the extrinsic curvature of the boundary, which forms part of the data for the Friedrich–Nagy system. However, it is clear that at least two more pieces of data are necessary to prescribe the gravitational radiation degrees of freedom. In the Friedrich–Nagy system, these two pieces of data are supplied by the combination (9.3) of the Weyl tensor components \( \Psi_0 \) and \( \Psi_4 \). However, the associated outgoing and ingoing null vectors are not determined by the local geometry but depend upon the choice of timelike evolution field \( T^a \) tangent to the boundary, according to (9.4). This could be avoided by requiring these null vectors to satisfy the local geometric condition that they be principal null directions of the Weyl tensor (cf [145]); but in a general spacetime, this would lead to four choices which would then have to be incorporated somehow into the evolution system. An alternative, suggested in [35], is to base the data on the eigenvector problem determined by the trace-free part of the extrinsic curvature of the boundary,

\[
(K_{ab} - \frac{1}{2} H_{ab} K)V^b = \lambda H_{ab} V^b. \quad (12.1)
\]
As in the preceding presentation, $H_{ab}$ is the intrinsic metric of the boundary. For a spherical worldtube $r = R$ in Minkowski space,

$$K_{ab} - \frac{1}{3}H_{ab}K = \frac{1}{3R}(H_{ab} + 3\tilde{T}_a\tilde{T}_b), \quad (12.2)$$

where $\tilde{T}_a$ is a timelike eigenvector. This raises the possibility of whether this eigenvector problem can be used to pick out a locally preferred timelike direction $\tilde{T}_a$ in the curved space case. Similar algebraic properties of the extrinsic curvature hold under roundness conditions which are typically satisfied by the artificial outer boundary of an isolated system. However, whether such an approach can be incorporated into the evolution system and whether the two radiation degrees of freedom can be encoded in the extrinsic curvature are not obvious.

Neither of the two strongly well-posed formulations of the IBVP described in sections 9 and 10 are based upon purely local geometric data. In both of them, a foliation of the boundary consistent with a choice of evolution field plays an essential nonlocal role. This suggests that a version of geometric uniqueness based upon purely local data might not be possible. The prescription of an evolution field $t^a$ as part of the boundary data provides the necessary structure to pose a version of geometric uniqueness [36, 34]. As explained in sections 4 and 5, the flow of the evolution field carries the initial edge $B_0$ into a foliation $B_t$ of the boundary, and it carries the initial Cauchy data into a stationary background metric $\tilde{g}_{ab}$ according to (5.12). Thus, the evolution field provides the two essential structures to geometrize the boundary data: the foliation $B_t$ determines the outgoing null direction $K^a$ and the preferred background metric allows the Sommerfeld derivative to be expressed covariantly as $K^a\nabla_a$ in terms of the background connection. Under a diffeomorphism, the evolution field transforms according to $t^a \rightarrow \psi_t^a t^a$ with the consequence that $\tilde{g}_{ab} \rightarrow \psi^* \tilde{g}_{ab}$.

The boundary data $q^a$ and $\sigma$ for the covariant version of the covariant Sommerfeld conditions (10.17)–(10.23) then have the geometric interpretation that

$$q^a = K^b(\nabla_b - \tilde{\nabla}_b)K^a \quad (12.3)$$

is the acceleration of the outgoing null vector $K^a$ relative to the background acceleration, and

$$\sigma = \frac{1}{2}Q^a Q^b (\nabla_a - \tilde{\nabla}_a)K_b \quad (12.4)$$

is the shear of $K^a$ relative to the background. The use of the shear in posing geometrical boundary conditions for the harmonic formulation was also suggested in [102]. The rotation freedom in the dyad dependence (12.4) can be removed by introducing the rank-2 shear tensor

$$\sigma^{ab} = \frac{1}{2}Q^{ac} Q^{bd} - \frac{1}{4}Q^{ab}Q^{cd} (\nabla_c - \tilde{\nabla}_c)K_d, \quad \sigma = Q_a Q_b \sigma^{ab}, \quad (12.5)$$

with $\sigma^{ab}\nabla_c = 0$.

By construction, all quantities involved in the boundary conditions map as tensor fields under a diffeomorphism $\psi$. As a result of the covariant form of the generalized harmonic equations (10.10) and (10.11), the solution $f_{ab} = g_{ab} - \tilde{g}_{ab}$ also maps as a tensor field. The metric $g_{ab}$ satisfies the generalized harmonic condition (10.12) with respect to the background $\tilde{g}_{ab}$ and the mapped metric $\psi^*g_{ab}$ satisfies the generalized harmonic condition with respect to $\psi^*\tilde{g}_{ab}$.

This can be taken one step further [34]. As characterized in [40], the Cauchy data $h_{ab}$ and $k_{ab}$ can be interpreted as the fields $\tilde{h}_{ab}$ and $\tilde{k}_{ab}$ on a disembodied 3-manifold $\tilde{S}_0$ via its embedding $\tilde{S}_0$ in the four-dimensional spacetime manifold $M$. A similar approach applies to the boundary data. Let

$$q^a = q_N N^a + q^a_T, \quad (12.6)$$

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so that $q^T_a$ is tangent to the boundary $T$. Then the fields $q_N$, $q^T_a$ and $\sigma^{ab}$ are intrinsic to the boundary. Along with the Cauchy data and the hyperbolic angle $\Theta$ at the edge $B_0$, they can be induced by the embedding of a disembodied version of data. This leads via the well-posedness of the IBVP with Sommerfeld data to a harmonic version of a

**Geometric uniqueness theorem.** Consider the 3-manifolds $\tilde{T}$ and $\tilde{S}_0$ meeting in an edge $\tilde{B}_0$. On $\tilde{S}_0$ prescribe the symmetric tensor fields $\tilde{h}_{ab}$ and $\tilde{k}_{ab}$, subject to the Hamiltonian and momentum constraints and the condition that $h_{ab}$ be a Riemannian metric. On $\tilde{B}_0$ prescribe the scalar field $\tilde{\Theta}$. On $\tilde{T}$ prescribe a smooth foliation $\tilde{B}_t$, parametrized by a scalar function $\tilde{t}$, the scalar field $\tilde{q}_N$, the vector field $\tilde{q}^T_a$ and the rank-2 tensor field $\tilde{\sigma}^{ab}$. Then, after embedding $\tilde{S}_0 \cup \tilde{T}$ as the boundary $S_0 \cup T$ of a 4-manifold $M$ as depicted in figure 1, this provides the Sommerfeld boundary data for a vacuum spacetime in a neighborhood of $B_0$ which is unique up to diffeomorphism.

Because the boundary data contain gauge information, this version of geometric uniqueness is weaker than for the Cauchy problem. It is an open question whether the boundary data can be prescribed purely in terms of local geometric objects [35]. Note that the data contain no information about the 3-metric of the boundary, not even that it is a timelike 3-manifold. The geometrical interpretation of the data involves the metric of the embedded spacetime, whose existence is in the content of the theorem. The diffeomorphism freedom lies in the freedom in the embedding and in the choice of evolution field $t^a$, which determines the gauge and background geometry. See [37] for a discussion of these issues in the context of linearized gravitational theory.

The spatial locality of the solution can be extended, say to a boundary with spherical topology, by patching solutions together. However, the locality in time presents a more complicated problem regarding the maximal development of the solution. For instance, the time foliation might develop a gauge pathology which prematurely stops the evolution. That makes it unclear how the maximal development for the Cauchy problem, as constructed by Choquet-Bruhat [147], might be generalized to the IBVP. A restart of the evolution at an intermediate time in order to extend the solution would introduce a new gauge, new initial data, a new evolution field and thus a new background metric. A maximal development based upon the original background would have to be based upon a maximal choice of evolution field.

The geometric nature of the Sommerfeld conditions (10.17)–(10.20) allows them to be formally applied to any metric formulation. In a $3+1$ formulation, the metric has the decomposition

$$g_{\mu\nu} = -n_\mu n_\nu + \tilde{N}_\mu \tilde{N}_\nu + Q_{\mu\nu},$$

(12.7)

where $\tilde{N}_\mu$ is the unit normal to the boundary which lies in the Cauchy hypersurfaces and, as before, $Q_{\mu\nu} = \tilde{Q}_{\mu\nu}$ is the 2-metric intrinsic to its foliation $B_t$. The Sommerfeld boundary conditions (10.17), (10.18) and (10.20) supply boundary data for the $N^\nu \kappa_{\mu\nu}$, $Q^\mu N^\nu k_{\mu\nu}$ and $Q^\mu Q^\nu k_{\mu\nu}$ components of the extrinsic curvature of the Cauchy foliation. However, (10.19) supplies the boundary data for the normal component of the shift, which for many $3+1$ formulations would require a Dirichlet condition that fixes its sign. The remaining Sommerfeld boundary conditions (10.21)–(10.23), which enforce the harmonic constraints, would also require modification depending upon the particular $3+1$ gauge conditions. See [75] for a discussion relevant to the BSSN formulation. Numerical tests would be necessary to study whether application of (10.17), (10.18) and (10.20) would improve the performance over the present boundary treatment of $3+1$ systems.
13. Numerical tests

Post and Votta [25] have emphasized that ‘Verification and validation establish the credibility of code predictions. Therefore it’s very important to have a written record of verification and validation results.’ The validation of a code implies that its predictions are in accord with observed phenomena. For the present status of numerical relativity, in the absence of any empirical observations, the burden falls completely on verification. Post and Votta list five verification techniques.

(1) ‘Comparing code results with an exact answer’.
(2) ‘Establishing that the convergence rate of the truncation error with changing grid spacing is consistent with expectations’.
(3) ‘Comparing calculated with expected results for a problem especially manufactured to test the code’.
(4) ‘Monitoring conserved quantities and parameters, preservation of symmetry properties and other easily predictable outcomes’.
(5) ‘Benchmarking—that is, comparing results from those with existing codes that can calculate similar problems’.

The importance of the first four techniques has now been recognized by most numerical relativity groups and their implementation in practice has improved the integrity of the field. Individual groups cannot easily carry out the fifth technique independently. This was the motivation behind formation of the Apples with Apples (AwA) Alliance [148].

The early attempts at developing numerical codes were primarily judged by their ability to simulate black holes, understandably because of the astrophysical importance of quantifying that system. When the difficulty with numerical stability became apparent, there was increased focus on a better mathematical and computational understanding of the analytic and numerical algorithms. Only a few groups had based their codes upon symmetric or strongly hyperbolic formulations of Einstein’s equations and fewer had even begun to worry about how to apply boundary conditions. The cross fertilization between computational mathematics and numerical relativity was entering a productive stage. At the same time, standardized tests were developed by the AwA Alliance in order to isolate problems, calibrate accuracy and compare code results, http://www.ApplesWithApples.org.

Such testbeds have been historically used in computational hydrodynamics. There are two fundamentally different types. One compares simulations of a physically important process, such as the binary black hole problem. The second type involves idealized situations which isolate problems, such as the ‘shock tube’ test in computational fluid dynamics. This is the type of testbed considered by the AwA Alliance.

The first tests were designed to study evolution algorithms in the absence of boundaries [149, 150]. Five tests were based upon a toroidal 3-manifold (equivalent to periodic boundary conditions).

- The robust stability test evolves random initial data in the linearized regime. This is a pass/fail test designed as a screen to eliminate unstable codes.
- The linearized wave test propagates a periodic plane wave either parallel or diagonal to an axis of the 3-torus. The test checks the accuracy in tracking both the amplitude and phase of the wave.
- The gauge wave test is a pure gauge version of the linearized wave test, but with amplitude in the nonlinear regime.
• The **shifted gauge wave** test is based upon a gauge wave with non-vanishing shift. Both the gauge wave and shifted gauge wave tests are challenging because of exponentially growing modes in the analytic problem [31].

• The **Gowdy wave** test simulates an expanding or contracting toroidal spacetime, which contains a plane-polarized gravitational wave in a genuinely curved, strong-field context.

The wave tests provide exact solutions which allow convergence measurements. Instabilities are monitored by the growth of the Hamiltonian constraint. Test results were carried out for codes based upon numerous formulations: harmonic, Friedrich–Nagy, NOR and several versions of BSSN and ADM. See [150] for the test results.

Tests of the Cauchy evolution algorithm cull out algorithms whose boundary stability is doomed from the outset. A subsequent plan for boundary tests was formulated by opening up one axis of the 3-torus to form a manifold with boundary. This has the advantage that the boundaries are smooth 2-tori, thus avoiding the complication of sharp boundary points. This could later be extended to opening up all three axes to test performance with a cubic boundary. For the robust stability test, the boundary data consist of random numbers. For the wave tests, the boundary data are supplied by the exact (or linearized) solution. See [148] for the detailed specifications of the five AwA boundary tests.

These boundary tests were first formulated and applied in the early development of boundary algorithms for harmonic codes. The robust stability test [76] was used to verify the stability of a code based upon a well-posed IBVP for linearized harmonic gravity [77]. Subsequently, the gauge wave tests were carried out with a harmonic code whose underlying IBVP was well-posed for homogeneous Dirichlet and Neumann conditions [13, 103]. This revealed problems in the very nonlinear regime, where the approximation of small boundary data was violated. The shifted gauge wave test posed an additional difficulty, beyond the unstable analytic modes that already challenged the Cauchy evolution test [31, 151]. The periodic time variation of the shift produced an effective oscillation of the boundaries which blue-shifted and trapped the error resulting from the reflecting boundary conditions. This led to unstable behavior in the nonlinear regime.

After formulation of the strongly well-posed harmonic IBVP described in section 10, the Sommerfeld boundary conditions were implemented and tested in a harmonic code [152–155]. Numerical stability and accurate phase and amplitude tracking were confirmed by the robust stability and linearized wave tests. An important attribute of strong well-posedness is the estimate of boundary values provided by the energy conservation obeyed by the principal part of the equations. This boundary stability extends to the semi-discrete system obtained by replacing spatial derivatives by finite differences obeying SBP (the discrete counterpart of integration by parts), so that energy conservation carries over to the semi-discrete problem [156]. Stability then extends to the fully discretized evolution algorithm obtained with an appropriate time integrator, such as Runge–Kutta [157]. It was found that these discrete conservation laws were both effective and essential in controlling the exponential analytic modes latent in the gauge wave test. Although the analytic proof of well-posedness given in [18] was based upon a scalar-wave energy differing by a small boost from the standard energy, it is interesting that these successful code tests were based upon the standard energy. This confirms the robustness of the underlying approach.

The oscillating boundaries in the shifted gauge wave test excite a different type of long-wavelength instability which could not be suppressed by purely numerical techniques. Knowledge of the Sommerfeld boundary data allows the wave to enter and leave the boundaries, but the numerical error, although small and convergent, excites an exponential mode of the analytic problem. However, because this instability violates the harmonic constraints, it was possible to suppress it by a harmonic constraint adjustment of the form (2.12) [31, 152]. This
example emphasizes the importance of understanding instabilities in the analytic problem in order to control them in a numerical simulation.

Other wave solutions which have been used for numerical tests are the Teukolsky waves [158], which are linearized spherical waves appropriate for testing a spherical boundary, and the nonlinear Brill waves [160], which are useful for testing wave propagation during collapse to a black hole. Teukolsky wave tests of the harmonic Sommerfeld conditions confirm that the constraint violation error due to homogeneous outer boundary data drops to numerical truncation error as the wave propagates off the grid [154]. Furthermore, when constraint damping is applied to the interior of the grid, the error drops to machine round-off. For Brill wave tests with the same code, homogeneous Sommerfeld conditions lead to considerable back reflection off the boundary, as expected from the discussion in section 8. In [159], Teukolsky waves were also used to test an implementation of the improved higher order harmonic boundary conditions proposed by Buchman and Sarbach [100].

Rinne, Lindblom and Scheel [98] have developed a numerical test for comparing back reflection of waves from a spherical boundary. First, using perturbative techniques, they construct a reference solution for a linearized gravitational wave propagating on an exterior Schwarzschild background. Then the full numerical code is run with a finite spherical outer boundary. The error with respect to the reference solution is used to compare different choices of boundary conditions. Using the first-order harmonic code described in [161], they used this test to compare several boundary conditions. The comparisons of homogeneous Sommerfeld boundary conditions were in accord with the theoretical expectations discussed in sections 8 and 10. The higher order Sommerfeld conditions and the $\Psi_0$ freezing condition both produced less back reflection than the first-order conditions (10.27)–(10.30). The test was also used to reveal the spurious effects arising from a sponge boundary condition and also from the combination of numerical dissipation and spatial compactification used by Pretorius [28, 29]. In an independent follow-up of this test [102], the advantages of higher order Sommerfeld conditions were confirmed.

Although 3 + 1 codes have been predominant in binary black hole simulations, boundary tests have not been very extensive as compared to harmonic codes. This is especially pertinent for the BSSN system. Boundary tests based on a gravitational wave perturbation of the Schwarzschild exterior have been carried out for the KST system [96]. The results revealed instabilities although they showed how improvements to the boundary conditions could reduce constraint violation. The robust stability and Brill wave tests have been applied to boundary conditions for a symmetric hyperbolic version of the Einstein–Christoffel system [93]. Although the Cauchy problem for this system is well-posed, both tests revealed instabilities due to the boundary algorithm. Again the tests were useful guides for understanding the problems with the boundary treatment.

Bona and Bona-Casas [162] have made the first application of the Gowdy wave boundary test. They show how it can be applied to a symmetric hyperbolic version of the first-order Z4 formalism. Here, as in many other studies, the Cauchy problem is well-posed but the strong well-posedness of the IBVP depends on the boundary condition. Improper boundary conditions can lead to instability and/or constraint violation. They first demonstrate that the test is effective at investigating methods for preserving the energy constraint for the Z4 system in a strong-field environment. In a subsequent work [163], they apply both the Gowdy wave and robust stability boundary tests in an expanded study of constraint violation in the Z4 framework. The robust stability case is applied both with opening up one axis of the 3-torus and with a fully cubic boundary. This allows testing SBP algorithms at the corners and edges. The results show numerical stability of the proposed boundary algorithms in the linearized regime. The Gowdy wave test extends this study to constraint preservation in the nonlinear
regime. The results provide further evidence of numerical stability and show that constraint violation can be kept at the level of discretization error.

14. Open questions

The IBVP has analytical, computational, geometrical and physical aspects. The analytic goal is a strongly well-posed IBVP, which is the prime necessity for the computational goal of an accurate evolution algorithm. It is also the raison d'être for the geometric goal of a gauge-invariant formulation of the boundary data. The prime physical goal, at present, is the accurate simulation of binary black holes. The binary black hole problem has taken a course of its own, which has been remarkably successful in view of the gaps in our current understanding of the other aspects of the IBVP.

Some important open questions which would help close those gaps are as follows.

• **Question 1.** Is there a strongly well-posed IBVP based upon a $3 + 1$ formulation?

Some insight into this question would be provided by the answer to

• **Question 2.** Can the necessary boundary data be represented by gauge-invariant, local geometric objects?

In the Friedrich–Nagy treatment, there are three pieces of boundary data which are not pure gauge: the trace $K$ of the extrinsic boundary curvature, which determines the location of the boundary, and the Weyl curvature components encoding the two radiation degrees of freedom. In the harmonic system, the Sommerfeld data which encode the radiation consist of the shear, or the Weyl curvature components for a higher order condition. This leads to

• **Question 3.** In the harmonic formulation, can the trace $K$ be used as gauge-invariant boundary data?

For the Cauchy problem, there exists a maximal development of the solution [147].

• **Question 4.** What is the proper formulation of the maximal development of the IBVP?

The quote of Turing at the beginning of this review expresses the relative degree of difficulty between the Cauchy problem and the IBVP.

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