

UNIVERSITY OF SOUTHAMPTON
FACULTY OF ENGINEERING, SCIENCE & MATHEMATICS
SCHOOL OF MATHEMATICS



The Construction of Boundary Conditions for
Electromagnetic Analogues of Formulations used
in Numerical Relativity

By
Christopher Richard Thomas Nunn

A thesis submitted for the degree of Master of Philosophy

December 2005

UNIVERSITY OF SOUTHAMPTON

ABSTRACT

FACULTY OF ENGINEERING, SCIENCE & MATHEMATICS

SCHOOL OF MATHEMATICS

Master of Philosophy

THE CONSTRUCTION OF BOUNDARY CONDITIONS FOR
ELECTROMAGNETIC ANALOGUES OF FORMULATIONS

USED IN NUMERICAL RELATIVITY

by Christopher Richard Thomas Nunn

This thesis investigates the construction of maximally dissipative and constraint preserving boundary conditions for electromagnetic analogues of two formulations presently used in numerical relativity. Accurate simulations of astrophysical situations either require correct boundaries to be applied or for these boundaries to be pushed out far enough that they are not causally connected to the region of interest. This work looks to tackle the first problem, considering electromagnetism in an attempt to construct general concepts that would transfer directly to formulations of the Einstein equations used in numerical relativity.

The early sections of the thesis introduce in a general way the requirements for continuum problems and their discretisations and the properties of maximally dissipative and constraint preserving boundary conditions. Consideration is then made of the advantages and limitations of using formulations of the Maxwell equations as analogues to formulations used in numerical relativity, before the introduction of the two formulations: KWB and Z1, that will be considered in this thesis.

The basic examples of the first order in space and second order in space wave equation, with and without shift, are used to help construct the boundary conditions for KWB and Z1. Where possible the energy method is used to analytically prove stability for the resulting schemes, which are then tested numerically.

Contents

1	Introduction	9
1.1	Motivation	9
1.2	Numerical relativity	10
1.3	Aim of research	11
2	The Continuum Initial Boundary Value Problem	13
2.1	Initial value problem	13
2.2	Initial boundary value problem	15
2.3	Well-posedness and strong hyperbolicity	16
2.3.1	Strong hyperbolicity and characteristic variables	16
2.3.2	Strong hyperbolicity sufficient & necessary for well-posedness	17
2.4	Characteristic variables of the wave equation	21
2.5	Maximally dissipative boundary conditions	23
2.6	Constraint preserving boundary conditions	26
3	Finite Differencing	29
3.1	Discrete stability and convergence	29
3.2	Semi-discrete boundaries	30
3.2.1	The second order in space wave equation	31

4	3+1 Formulations of General Relativity	33
4.1	The 3+1 split	33
4.2	Adapting the Einstein equations	37
4.2.1	Evolution of the Einstein equations	37
4.2.2	The ADM system	38
4.2.3	The BSSN system	39
4.2.4	The NOR system	39
4.2.5	The Z4 system	40
5	Electromagnetism	42
5.1	Electromagnetic analogues of formulations of general relativity . .	42
5.2	The Maxwell equations	42
5.3	The KWB system	45
5.4	The Z1 system	49
6	KWB	53
6.1	Discrete energy	53
6.1.1	Discrete energy without boundaries	53
6.1.2	Positive definite discrete energy without boundaries	54
6.1.3	Lower order terms	55
6.1.4	Discrete energy with a boundary	56
6.1.5	Positive definite discrete energy with a boundary	58
6.2	Constraint preserving boundary conditions for the KWB system .	61
6.3	The KWB system with shift	62
6.3.1	Exact solution for the KWB system with shift	63
6.3.2	MDBC for the KWB system with shift	67
6.3.3	CPBC for the KWB system with shift	68

6.3.4	The second order in space wave equation with shift	69
6.3.5	Constructing an energy for the KWB system with shift . . .	73
6.4	KWB numerical results	75
6.4.1	KWB experimental setup	75
6.4.2	Stability tests	75
6.4.3	Convergence testing	80
7	The Z1 System	85
7.1	Energy without boundaries	85
7.2	Discretisation of the Z1 system	86
7.3	Discrete boundaries for the Z1 system	89
7.3.1	Decomposition of the Z1 system into wave equations . . .	89
7.3.2	The first order in space wave equation	90
7.3.3	Numerical results for the first order wave equation	94
7.3.4	The second order in space wave equation	96
7.4	Semi-discrete boundary conditions for the Z1 system	97
7.5	Numerical results for the Z1 system with boundaries	98
8	Conclusions	109
A	Derivations	112
A.1	Definitions of the extrinsic curvature	112
A.2	The Gauss equation	113
A.3	The Codazzi equation	115
A.4	The Hamiltonian constraint	115
A.5	The momentum constraint	116
A.6	The evolution equation of the extrinsic curvature	117

B	Electromagnetic 3+1 Split	121
C	Summation by Parts	123
D	Scalar Product and Norm	124
D.1	The Cauchy-Schwarz inequality	124
D.2	The triangle inequality	125
D.3	The complex square	125

Acknowledgements

I would like to thank my supervisor, Carsten Gundlach, for his eternal patience as well as for his insight and guidance, without which I would have been lost.

I would also like to thank my advisor, James Vickers, for his continued support during my time here.

My gratitude to my family for always encouraging me throughout my research.

Many thanks go to my brother and David Hilditch for proof reading.

My appreciation for the financial support of EPSRC.

Finally, my appreciation to the Southampton University GR group as a whole for making my time here very special and a unique experience.

Definitions & Abbreviations

ODE	Ordinary differential equation
PDE	Partial differential equation
KWB	Knapp, Walker, Baumgarte formulation of electromagnetism
MDBC	Maximally dissipative boundary conditions
CPBC	Constraint preserving boundary conditions
ADM	Arnowitt, Deser, Misner formulation of general relativity
BSSN	Baumgarte, Shapiro, Shibata, Nakamura formulation of general relativity
NOR	Nagy, Ortiz, Reula formulation of general relativity
\doteq	Equal to on the boundary
$(u_i, v_i) = h \sum_i u_i^\dagger v_i$	Scalar product of u_i and v_i
$\ u\ ^2 = (u, u)$	l_2 norm of u unless otherwise stated
i, j, k	Latin indices indicate 1, 2, 3
μ, ν	Greek indices indicate 0, 1, 2, 3
$u_{,t} = \partial_t u$	The derivative of u with respect to t
U^0	U at the gridpoint 0
\dot{U}	Time derivative of U
E_i^2	$E_i E^i$

Chapter 1

Introduction

1.1 Motivation

One of the well-known and important scientific and technological aims at the present time is the detection of gravitational waves from astrophysical events such as the inspiral and coalescence of binary black holes. Traditional techniques can be used to describe the orbiting black holes before coalescence and the perturbed black hole that results after coalescence but the period in between these phases can, at present, only be tackled with numerical relativity, i.e. computer simulations of these astrophysical scenarios. With an accurate and stable simulation, a gravitational waveform could be extracted from the numerical solution at late times, providing a template that could be used in matched filtering techniques to obtain a gravitational signal from observational data received by gravitational wave detectors. Templates will also help in the interpretation of such a signal, providing information about the event from which the gravitational signal originated.

Numerical relativists try to simulate astrophysical situations by evolving given initial and/or boundary data. For this purpose, the 3+1 split of the Einstein equations can be used, which provides a number of evolution equations, meaning that we can provide physical initial data and evolve forward in time, applying boundary data if necessary. The problems that hinder these simulations include those associated with stability, in particular with reference to boundary conditions. A stable scheme is vital for long-term simulations as instabilities can end the simulation with small numerical errors growing to swamp the solution. Con-

sistent boundary conditions are equally important to the simulation, as errors can equally well enter the domain from the boundary.

1.2 Numerical relativity

When the 3+1 split mentioned above is made, spacelike hypersurfaces and a time coordinate are introduced on the space-time and the Einstein equations decompose into evolution equations, which involve time derivatives of the evolution variables, and constraint equations on the spacelike hypersurfaces. Considering the ‘hyperbolicity’ of the evolution equations allows statements to be made about the well-posedness of the problem in question, which is related to the continuity of the solution with respect to the initial data. For a formulation to be useful, it must be well-posed and a lot of effort in numerical relativity has gone into reworking the Einstein equations into formulations that are well-posed at the continuum and hence allow the possibility of a stable numerical discretisation.

One of the original formulations used in numerical relativity was the ADM system. Now it has been shown, for example in [1], that the first order reduction of ADM is not well-posed with a densitised lapse gauge condition, i.e. with the lapse gauge variable as a certain function of coordinates. Most of the instability problems experienced in evolutions when this formulation was used can generally be attributed to this property. Once this was understood, modifications were made to the ADM formulation in an attempt to determine some formulations that would be well-posed. Two formulations that came about from these modifications were the BSSN and NOR systems. The BSSN system was constructed by both Shibata and Nakamura [2] and Baumgarte and Shapiro [3] by introducing three connection functions into the ADM system and adding multiples of the constraint equations to the evolution equations. The NOR system, introduced by Nagy, Ortiz and Reula,[1] also has new variables, related to those introduced into the BSSN system, and a multiple of a constraint added to an evolution equation. A third formulation that was constructed in a different way is the Z4 system, introduced by Bona, Ledvinka, Palenzuela and Z’acek.[4] In this system, a new variable is introduced into the field equations before making a 3+1 split. These formulations give improved stability in numerical simulations and alongside other reformulations, they have allowed people to concentration on other problems such as boundary conditions.

Although the problems of well-posedness and stability have not been completely resolved in the absence of boundaries, one of the major problems faced today is to keep these properties when artificial boundary conditions are introduced. We need to be able to prescribe boundary conditions and a discretisation of the derivatives on the boundary so that we retain well-posedness and stability. A lot of work in the field is done by pushing the boundary out far enough that it is causally disconnected to the region of interest. However, even with the assistance of multi-grids and the resulting higher resolution, it is still a waste of computational resource that could be utilised in the region of interest.

1.3 Aim of research

The main aim of this research is to obtain some general methods for applying boundaries to an evolution scheme such that the continuum problem is well-posed and the solution of the discrete scheme converges to the continuum solution. Two representative formulations used in numerical relativity are the NOR and Z4 systems and both of these systems have analogues in electromagnetism, i.e. the 3+1 split of the Maxwell equations can be written in a similar structure to these formulations of the Einstein equations with an explicit term-by-term comparison. It is useful to analyse these analogues - the KWB and Z1 systems - due to their relative simplicity and the presence of an exact solution for electromagnetism.

Boundary conditions prescribed for these electromagnetic schemes may give insight into how the generalised boundaries may work for numerical relativity. The electromagnetic formulations will be broken down into systems of equations that can be compared to the first order in time, first order in space wave equation and the first order in time, second order in space wave equation so that simple techniques can be consistently combined to give a full prescription for the boundaries. Both maximally dissipative boundary conditions and constraint preserving boundary conditions will be considered. The former puts a limit on the characteristic variables (combinations of the evolution variables that travel at known speeds) that are coming into the grid. With this boundary condition, a bounded, positive definite energy, which includes the boundary, can often be found, which ensures stability of the scheme and hence convergence through the use of the Lax theorem. In addition to the main system energy, a constraint energy can also be constructed from the constraint variables and constraint preserving boundary

conditions work by ensuring that this constraint energy is non-increasing. Care must be taken to appreciate the limitations of these electromagnetic analogues but it is likely that the convergence of these boundary conditions in this situation is a necessary condition for them to work in full general relativity. It is also important that the continuum and discrete situations are kept distinct. The boundary conditions will be described at the continuum level first before a discretisation is made.

In chapter 2, we review initial value problems and initial boundary value problems, describing the general construction and giving some general properties of maximally dissipative boundary conditions and constraint preserving boundary conditions at the continuum. In chapter 3 we go on to describe the basic translation of continuum evolution equations and boundary conditions into semidiscrete ODE's. Chapter 4 follows the 3+1 split of the Einstein equations, giving the derivation of the ADM and subsequent construction of the BSSN, NOR and Z4 systems. In chapter 5, we begin to look at the formulations of electromagnetism that we will use to test our boundary prescription, introducing the KWB and Z1 system, before studying them both in depth in chapters 6 and 7, where we attempt to construct energies at the continuum and the discrete level and apply the boundary conditions mentioned above. We perform numerical tests on these formulations, with a zero shift and a non-zero shift, explaining the decomposition into the first order in space and second order in space wave equation that motivates our construction of boundary conditions. Finally we conclude with a review of the success of the various boundary conditions tested.

Chapter 2

The Continuum Initial Boundary Value Problem

2.1 Initial value problem

Stability and convergence are vital when discretising a set of equations into a numerical scheme. However, before a discretisation is made, the continuum problem must be well-posed. A problem is said to be well-posed if:

- a solution exists
- the solution is unique
- the solution depends continuously upon the initial data i.e. a small change in the initial data corresponds to a small change in the solution.

Considering a non-linear system, we can make a linearisation of the system and then the third point above is equivalent to saying that the norms of the perturbations of the solution and initial data must satisfy

$$\|\delta u(\cdot, t)\| \leq F(t)\|\delta u(\cdot, 0)\|, \quad (2.1)$$

where $F(t)$ does not depend upon the initial data. To justify the consideration of linear systems, the well-posedness of a linearised system is a necessary condition for well-posedness of the corresponding non-linear system.

When considering a linear system we can give a restriction on the norms of the solution and the initial data rather than the norms of the perturbations. With constant coefficients, we can write a definition of well-posedness

$$\|u(\cdot, t)\| \leq K e^{\alpha t} \|u(\cdot, 0)\|, \quad (2.2)$$

where K and α are independent of the initial data and $\|\cdot\|$ is an appropriate norm. Considering a simple first order differential equation with a lower order term and a constant coefficient α

$$u_t = u_x + \alpha u, \quad (2.3)$$

we can introduce the new variable

$$v = e^{-\alpha t} u, \quad (2.4)$$

so that

$$v_t = v_x \quad (2.5)$$

and hence we have

$$\|v(\cdot, t)\| = \|v(\cdot, 0)\| \quad (2.6)$$

and therefore the solution

$$\|u(\cdot, t)\| = e^{\alpha t} \|u(\cdot, 0)\|. \quad (2.7)$$

The K in equation (2.2) comes about when considering a system of equations.

We also need to relate the well-posedness of the variable coefficient case to the well-posedness of the constant coefficient case. We can make use of the frozen coefficients approximation to neglect variable coefficients; for example consider the Cauchy problem with variable coefficients

$$u_t(x, t) = P \left(x, t, \frac{\partial}{\partial x} \right) u(x, t) \quad (2.8)$$

for a first order system. Then we can look at all the systems where the coefficients are frozen to a constant value at an arbitrary point (x_0, t_0) . The frozen coefficients approximation states that if all of these constant coefficient problems are well-posed, then the variable coefficient problem is also well-posed.[5]

It is important to note that the choice of norm is important as a system can be well-posed with one norm and ill-posed with another and the standard L_2 norm is

not necessarily the right choice, as shown by the following example.[6] The wave equation written in second order in space form,

$$\dot{\phi} = \pi, \quad (2.9)$$

$$\dot{\pi} = \partial^i \partial_i \phi, \quad (2.10)$$

permits a family of initial data for which it is impossible to find K and α such that (2.2) is satisfied when using the L_2 norm:

$$\|u\| = \sqrt{\int |u|^2 dx} = \sqrt{\int (\pi^2 + \phi^2) dx}. \quad (2.11)$$

Considering the solution

$$\phi = \sin(\omega x) \cos(\omega t), \quad (2.12)$$

$$\pi = -\omega \sin(\omega x) \sin(\omega t), \quad (2.13)$$

ω can be increased arbitrarily and therefore the norm of the solution at time t cannot be bounded by the norm at $t = 0$.

Another way to look at the norm is to consider it as an energy. Later we will construct energies that are quadratic in the evolution variables of the systems we are considering and use the conservation of these energies to imply well-posedness. For this example of the second order in space wave equation, the ‘physical’ energy density is

$$\epsilon = \pi^2 + \partial^i \phi \partial_i \phi \quad (2.14)$$

and we have well-posedness for the wave equation in this norm. However, because we also want the norm we are using to be positive definite, we introduce a lower order term for ϕ

$$\|u\| = \sqrt{\int (\pi^2 + \phi^2 + \partial^i \phi \partial_i \phi) dx} \quad (2.15)$$

and again the wave equation is well-posed in this norm due to the presence of the first derivative of ϕ .

2.2 Initial boundary value problem

The definition of well-posedness for the initial value problem can be extended to an initial-boundary value problem by replacing ‘initial data’ with ‘initial data and boundary data’. So in addition to the conditions above, a small change in the boundary data must also give rise to only a small change in the solution.

We first look at the case of a system that is first order in time and first order in space

$$\partial_t u = P^i \partial_i u + Qu, \quad (2.16)$$

where u is a vector of N variables and P^i and Q are $N \times N$ matrices.

Note that we will be considering hyperbolic systems, i.e. those systems where the eigenvalues of the principal part P are real. When this is the case, we can calculate the eigenvectors of the principal part and this allows us to construct the characteristic variables of the system, which are combinations of the evolution variables that describe the incoming and outgoing data. We aim to introduce a boundary to a domain without losing the well-posedness of the system and this can be done using the characteristic variables. We need to be careful not to over-specify the problem by applying boundary conditions to the outgoing or zero-speed characteristic variables. It is important for hyperbolic problems that the number of boundary conditions imposed at a boundary should be equal to the number of incoming characteristics at that boundary.[7]

For simplicity, we begin with a linear system with constant coefficients (2.16) and introduce a direction n^i , which will later be taken to be the normal to the boundary. We define the projector q^i_j into the space that is normal to n_i

$$q^i_j \equiv \delta^i_j - n^i n_j \quad (2.17)$$

in order to decompose the derivatives into those in the direction of n_i and those transverse to n_i . We will use the notation A, B for indices that have been projected by q^i_j .

Hence

$$\partial_t u = P^n \partial_n u + P^B \partial_B u + Qu, \quad (2.18)$$

where $P^n = n_i P^i$.

2.3 Well-posedness and strong hyperbolicity

2.3.1 Strong hyperbolicity and characteristic variables

Consider P^n in equation (2.18). The definition of weak hyperbolicity states that P^n has real eigenvalues whilst strong hyperbolicity requires that P^n has real eigenvalues and a full set of eigenvectors. We will now show that strong hyperbolicity is a necessary and sufficient condition for well-posedness of an initial value problem.

As we are only interested in P^n , we consider the 1D case

$$\partial_t u = P \partial_x u + Qu. \quad (2.19)$$

For well-posedness, we require that a unique solution $u(t)$ exists and

$$\exists K, \alpha : \forall u(0) \quad \|u(t)\| \leq K e^{\alpha t} \|u(0)\| \quad (2.20)$$

for $t \geq 0$. We first analyse the case of (2.19) where $Q = 0$

$$\partial_t u = P \partial_x u. \quad (2.21)$$

The definition for strong hyperbolicity in this case is that the matrix P has real eigenvalues and a full set of eigenvectors. The second condition is equivalent to the matrix being diagonalisable as the matrix of eigenvectors T can be used to diagonalise P

$$T^{-1}PT = \Lambda, \quad (2.22)$$

where Λ is a diagonal matrix whose diagonal is constructed of the eigenvalues of P .

Theorem 2.3.1: *Strong Hyperbolicity of a first order 1D system of Partial Differential Equations is a necessary and sufficient condition for the well-posedness of the associated initial value problem*

2.3.2 Strong hyperbolicity sufficient & necessary for well-posedness

From above $T^{-1}PT = \Lambda$, and characteristic variables can be introduced

$$U = T^{-1}u. \quad (2.23)$$

Hence, substituting (2.23) into (2.21) gives

$$\begin{aligned} \partial_t(TU) &= P \partial_x(TU) \\ T \partial_t U &= PT \partial_x U \\ \partial_t U &= T^{-1}PT \partial_x U \\ \partial_t U &= \Lambda \partial_x U, \end{aligned} \quad (2.24)$$

which decouples the system into

$$\partial_t U^j = \lambda_j \partial_x U^j, \quad (2.25)$$

where j runs from 0 to N . Using a Fourier transform

$$U^j(x, t) = \frac{1}{\sqrt{2\pi}} \int_{\omega=-\infty}^{\infty} e^{i\omega x} \hat{U}^j(\omega, t) d\omega \quad (2.26)$$

and substituting this into (2.25) gives

$$\partial_t \hat{U}^j = i\omega \lambda_j \hat{U}^j, \quad (2.27)$$

of which the solution is

$$\hat{U}^j = e^{i\omega \lambda_j t} \hat{U}^j(\omega, 0). \quad (2.28)$$

Taking the L_2 norm of this solution and using Parseval's Relation

$$\|u\|^2 = \|\hat{u}\|^2, \quad (2.29)$$

the following is true

$$\begin{aligned} \|U^j(x, t)\|^2 &= \|\hat{U}^j(\omega, t)\|^2 \\ &= |e^{i\omega \lambda_j t}| \|\hat{U}^j(\omega, 0)\|^2 \\ &= |e^{i\omega \lambda_j t}| \|U^j(x, 0)\|^2. \end{aligned} \quad (2.30)$$

As the eigenvalues of P are real,

$$|e^{i\omega \lambda_j t}| = 1, \quad (2.31)$$

so

$$\|U^j(x, t)\|^2 = \|U^j(x, 0)\|^2 \quad (2.32)$$

and therefore

$$\|U(x, t)\|^2 = \|U(x, 0)\|^2. \quad (2.33)$$

Now, translating back into evolution variables

$$\begin{aligned} \|u(x, t)\|^2 &= \|TU(x, t)\|^2 \\ &\leq |T| \|U(x, t)\|^2 \\ &= |T| \|U(x, 0)\|^2 \\ &\leq |T| |T^{-1}| \|u(x, 0)\|^2. \end{aligned} \quad (2.34)$$

Therefore, we have the inequality for the definition of well-posedness with $K = |T| |T^{-1}|$ and $\alpha = 0$. When we consider a system that is not 1D, the diagonal matrix Λ and the matrix of eigenvectors T will be dependent upon the direction n_i and will be subscripted, Λ_n and T_n . This means that we can take $K = \sup_n (|T_n| |T_n^{-1}|)$ and we will need the supremum to be finite.

We now show that strong hyperbolicity is a necessary condition for well-posedness. Firstly, we show that well-posedness requires the eigenvalues to be real. Let ϕ be the eigenvector corresponding to the eigenvalue λ . A solution can be constructed,

$$u = e^{i\omega(\lambda t + x)}\phi, \quad (2.35)$$

with initial data

$$u(x, 0) = e^{i\omega x}\phi \quad (2.36)$$

so the L_2 norm of (2.35) gives

$$\|u(x, t)\| = e^{i\omega\lambda t}\|u(x, 0)\|. \quad (2.37)$$

Hence, writing $\lambda = a + ib$, well-posedness requires

$$\operatorname{Re}[(a + ib)(i\omega)] \leq \alpha \Rightarrow -b\omega \leq \alpha. \quad (2.38)$$

As ω is arbitrary, b must therefore equal zero and we are left with λ real.

Finally, assume there is not a full set of eigenvectors. Hence the Jordan canonical form will have at least one Jordan block of size greater than 1×1 . Consider the system of equations where P is the 2×2 Jordan block

$$\partial_t u = \begin{pmatrix} \lambda & 0 \\ 1 & \lambda \end{pmatrix} \partial_x u$$

where $u = (u^1, u^2)^T$. Therefore, performing a Fourier transform gives

$$\begin{pmatrix} \partial_t u^1 \\ \partial_t u^2 \end{pmatrix} = \begin{pmatrix} \lambda & 0 \\ 1 & \lambda \end{pmatrix} \begin{pmatrix} i\omega u^1 \\ i\omega u^2 \end{pmatrix},$$

from which the system can be written as

$$\dot{u}^1 = i\omega\lambda u^1 \quad (2.39)$$

$$\dot{u}^2 = i\omega\lambda u^2 + i\omega u^1. \quad (2.40)$$

Hence, the solution to (2.39) is as above

$$u^1(t) = e^{i\omega\lambda t}u^1(0), \quad (2.41)$$

whilst the solution to (2.40) can be given by

$$\begin{aligned} \dot{u}^2 - i\omega\lambda u^2 &= i\omega u^1 \\ \frac{d}{dt}(e^{-i\omega\lambda t}u^2) &= i\omega u^1 e^{-i\omega\lambda t} \\ &= i\omega u^1(0) \\ e^{-i\omega\lambda t}u^2 &= i\omega u^1(0)t + C \\ u^2(t) &= C e^{i\omega\lambda t} + i\omega u^1(0)t e^{i\omega\lambda t} \\ u^2(t) &= e^{i\omega\lambda t}u^2(0) + i\omega t e^{i\omega\lambda t}u^1(0). \end{aligned} \quad (2.42)$$

Therefore the solution u^2 can be made arbitrarily large by increasing the size of ω . For a larger Jordan block, continuing in the same way would give the solution for u^3 ,

$$u^3(t) = e^{i\omega\lambda t}u^3(0) + e^{i\omega\lambda t}u^2(0)(i\omega t - \omega^2 t^2) \quad (2.43)$$

and so on. This can be shown explicitly by considering a Jordan block A of size $N \times N$

$$\partial_t u = A \partial_x u. \quad (2.44)$$

Taking the Fourier transform as above gives

$$\partial_t \hat{u} = i\omega A \hat{u}. \quad (2.45)$$

Therefore the solution is

$$\hat{u}(t) = e^{i\omega t A} \hat{u}(0) \quad (2.46)$$

as

$$\begin{aligned} \partial_t \hat{u} &= \hat{u}(0) \partial_t \left[\sum_{j=0}^{\infty} \frac{1}{j!} i^j \omega^j t^j A^j \right] \\ &= i\omega A \hat{u}(0) \left[\sum_{j=1}^{\infty} \frac{1}{(j-1)!} i^{(j-1)} \omega^{(j-1)} t^{(j-1)} A^{(j-1)} \right] \\ &= i\omega A \hat{u}. \end{aligned} \quad (2.47)$$

We write the norm of the solution

$$\begin{aligned} \|u(t)\|^2 &= \|\hat{u}(t)\|^2 \\ &= |e^{i\omega t A}| \|\hat{u}(0)\|^2 \\ &= |e^{i\omega t A}| \|u(0)\|^2 \end{aligned} \quad (2.48)$$

and therefore, if we let $J = A - \lambda I$,

$$\begin{aligned} |e^{i\omega t A}| &= |e^{i\omega\lambda I t}| |e^{i\omega J t}| \\ &= |e^{i\omega J t}| \\ &= \left| \sum_{j=0}^{N-1} \frac{i^j \omega^j J^j t^j}{j!} \right|, \end{aligned} \quad (2.49)$$

which grows like $|\omega|^{N-1}$. Note that the N th power of an $N \times N$ matrix of the form J is zero. As an arbitrary matrix A can be put into Jordan canonical form, we know that if A does not have an N -dimensional eigenspace, its Jordan canonical form will have a Jordan block of size greater than one and the calculation above

shows that the problem will not be well-posed. Hence a full set of eigenvectors is needed for well-posedness.

Note that although we set $Q = 0$ at the start of this calculation, Theorem 4.3.2 in [7] states that perturbing this system with lower order terms does not affect the well-posedness.

2.4 Characteristic variables of the wave equation

As a simple example of calculating characteristic variables, we will find the characteristic variables of the wave equation in second order in space form. As we are going to be looking at first order in time, second order in space formulations, the wave equation in this form is an obvious starting point.

The wave equation

$$\ddot{\phi} = \phi_{,ii} \tag{2.50}$$

can be written in first order in time, second order in space form by introducing the variable $\pi = \partial_t \phi$:

$$\dot{\phi} = \pi \tag{2.51}$$

$$\dot{\pi} = \phi_{,ii} \tag{2.52}$$

and using the projection q_i^j to the space that is normal to n_i as above, this can be written as

$$\dot{\phi} = \pi \tag{2.53}$$

$$\dot{\pi} = \phi_{,nn} + \phi_{,BB}. \tag{2.54}$$

Now, we separate the evolution variables up into blocks

- π and $\phi_{,n}$
- $\phi_{,B}$.

For the first block

$$\partial_t \begin{pmatrix} \pi \\ \phi_{,n} \end{pmatrix} = \partial_n \begin{pmatrix} \phi_{,n} \\ \pi \end{pmatrix} + \partial_B \begin{pmatrix} \phi_{,B} \\ 0 \end{pmatrix},$$

so

$$P_n = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Now, from (2.23), we need the inverse of the matrix of eigenvectors so that we can transform the evolution variables to characteristic variables. However

$$P^\dagger(T^{-1})^\dagger = (T^{-1})^\dagger \Lambda \quad (2.55)$$

means that instead of calculating the eigenvectors of P^n and inverting this matrix, we can just calculate the transpose of the matrix of eigenvectors of P_n^\dagger to give us T_n^{-1} .

The eigenvalues of P_n^\dagger are $\lambda = \pm 1$, corresponding to the two eigenvectors:

$$\begin{pmatrix} 1 \\ 1 \end{pmatrix} \text{ and } \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

Hence, we can write down the characteristic variables:¹

$$U_\pm = \pi \pm \phi_{,n}. \quad (2.56)$$

For the second block

$$\partial_t(\phi_{,B}) = \partial_B \pi$$

and hence the other characteristic variables are zero speed

$$U_B = \phi_{,B}. \quad (2.57)$$

We should be careful to note here that any multiple of the transverse derivative $\phi_{,B}$ can be added to the characteristic variables due to commutation of partial derivatives. For example, if we alter U_+

$$U_+ = \pi + \phi_{,n} + \sum_B \phi_{,B}, \quad (2.58)$$

¹Note that in general the characteristic variables U_\pm are defined in terms of a normal pointing outward from a boundary, which prescribes U_+ to be an incoming characteristic variable at the boundary. For the work here, we will often be considering a 1D Cartesian grid and therefore we have adopted a slightly awkward convention for coding purposes of U_+ incoming at the right boundary and U_- incoming at the left boundary, keeping U_\pm travelling in their respective directions. In analytic calculations we will always talk about U_+ being the incoming characteristic but this may differ when coding issues arise.

the time derivative is

$$\begin{aligned}
\dot{U}_+ &= \phi_{,nn} + \phi_{,BB} + \pi_{,n} + \sum_B \pi_{,B} \\
&= (\pi + \phi_{,n} + \sum_B \phi_{,B})_{,n} + \text{transverse derivatives} \\
&= \partial_n U_+ + \text{transverse derivatives}.
\end{aligned} \tag{2.59}$$

so the evolution equation of the characteristic variable holds because $\phi_{,Bn} = \phi_{,nB}$ as we are considering $\phi_{,B}$ as a derivative and not as an auxiliary variable, in contrast to a fully first order reduction, where an auxiliary variable is introduced to replace the derivative.

2.5 Maximally dissipative boundary conditions

We can control the energy of the system by controlling the flux coming in and out of the domain at the boundary and we use maximally dissipative boundary conditions to do this.

Maximally dissipative boundary conditions involve specifying incoming characteristic variables in the following way:

$$U_+ = \kappa U_- + f, \tag{2.60}$$

where κ is a constant and f is free incoming data.

Consider the first order system of partial differential equations with constant coefficients

$$\partial_t u = P^i \partial_i u. \tag{2.61}$$

Strong hyperbolicity permits the construction of a symmetriser of P_n in the following way.

$$H_n = (T_n^{-1})^\dagger B_n T_n^{-1}, \tag{2.62}$$

where B_n is hermitian, positive definite and commutes with Λ_n . By construction H_n is hermitian and positive definite. If the symmetriser H_n is independent of the direction n_i , then we will call the system symmetric hyperbolic.

A positive definite energy density can be given

$$\epsilon = u^\dagger H u \tag{2.63}$$

and taking the time derivative gives

$$\begin{aligned}
\partial_t \epsilon &= (\partial_t u^\dagger) H u + u^\dagger H \partial_t u \\
&= \partial_i (u^\dagger P^{i\dagger}) H u + u^\dagger H \partial_i (P^i u) \\
&= \partial_i u^\dagger H P^i u + u^\dagger H P^i \partial_i u \\
&= \partial_i (u^\dagger H P^i u),
\end{aligned} \tag{2.64}$$

where, because we have a total divergence, we can specify the flux

$$F^i = u^\dagger H P^i u. \tag{2.65}$$

The energy is the integral over the domain of the energy density

$$E = \int_{\Omega} \epsilon dV \tag{2.66}$$

and its differential is

$$\frac{dE}{dt} = \int_{\Omega} \partial_i F^i dV, \tag{2.67}$$

$$= \int_{\partial\Omega} F^i ds_i, \tag{2.68}$$

where ds_i is the surface element on the boundary $\partial\Omega$. The first equality comes from (2.64) and the second from Gauss' Law. This can be rewritten

$$\begin{aligned}
\frac{dE}{dt} &= \int_{\partial\Omega} u^\dagger H P^n u ds \\
&= \int_{\partial\Omega} U^\dagger T^\dagger H P^n T U ds,
\end{aligned} \tag{2.69}$$

where n_i is normal and outward-pointing with respect to $\partial\Omega$. Recall the definition of B ,

$$B = \begin{pmatrix} B_+ & 0 & 0 \\ 0 & B_- & 0 \\ 0 & 0 & B_0 \end{pmatrix},$$

where the B_+ , B_- and B_0 correspond to the positive, negative and zero eigenvalues respectively. Therefore

$$\begin{aligned}
\frac{dE}{dt} &= \int_{\partial\Omega} U^\dagger B \Lambda U \\
&= \int_{\partial\Omega} F^n ds, \quad F^n = U^\dagger B \Lambda U.
\end{aligned} \tag{2.70}$$

Writing

$$\Lambda = \begin{pmatrix} \Lambda_+ & 0 & 0 \\ 0 & \Lambda_- & 0 \\ 0 & 0 & \Lambda_0 \end{pmatrix},$$

we have

$$F^n = \begin{pmatrix} U_+^\dagger & U_-^\dagger & U_0^\dagger \end{pmatrix} \begin{pmatrix} \Lambda_+ B_+ & 0 & 0 \\ 0 & \Lambda_- B_- & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} U_+ \\ U_- \\ U_0 \end{pmatrix}$$

and hence

$$F^n = U_+^\dagger \Lambda_+ B_+ U_+ + U_-^\dagger \Lambda_- B_- U_- \quad (2.71)$$

To give a bounded energy, maximally dissipative boundary conditions can be used, where L is now the coupling matrix between the ingoing and the outgoing vectors of characteristic variables. First consider the case where $f = 0$. Substituting the maximally dissipative boundary condition into (2.71) gives

$$F^n = U_-^\dagger L^\dagger B_+ \Lambda_+ L U_- + U_-^\dagger B_- \Lambda_- U_- \quad (2.72)$$

Therefore a way of ensuring a decreasing energy in (2.70) is to force F^n to be negative. To enforce this, we need

$$M = L^\dagger B_+ \Lambda_+ L + B_- \Lambda_- \quad (2.73)$$

to be negative definite. Now consider the case where $f \neq 0$. Again, the maximally dissipative boundary condition can be substituted into (2.71) giving

$$\begin{aligned} F^n &= U_-^\dagger L^\dagger B_+ \Lambda_+ L U_- + U_-^\dagger B_- \Lambda_- U_- \\ &\quad + U_-^\dagger L^\dagger B_+ \Lambda_+ f + f^\dagger B_+ \Lambda_+ L U_- + f^\dagger B_+ \Lambda_+ f. \end{aligned} \quad (2.74)$$

Now the function g is introduced, defined as

$$g = M^{-1} L^\dagger B_+ \Lambda_+ f. \quad (2.75)$$

The expression

$$(U_-^\dagger + g^\dagger) M (U_- + g) \quad (2.76)$$

is negative as M is negative definite. This expression can be expanded

$$\begin{aligned} (U_-^\dagger + g^\dagger) M (U_- + g) &= U_-^\dagger M U_- + U_-^\dagger L^\dagger B_+ \Lambda_+ f + f^\dagger \Lambda_+ B_+ L U_- \\ &\quad + f^\dagger \Lambda_+ B_+ L M^{-1} M M^{-1} (L^\dagger B_+ \Lambda_+ L + B_- \Lambda_-) L^{-1} f \\ &\quad - f^\dagger \Lambda_+ B_+ L M^{-1} B_- \Lambda_- L^{-1} f \\ &= U_-^\dagger M U_- + U_-^\dagger L^\dagger B_+ \Lambda_+ f + f^\dagger \Lambda_+ B_+ L U_- \\ &\quad + f^\dagger B_+ \Lambda_+ f - f^\dagger \Lambda_+ B_+ L M^{-1} B_- \Lambda_- L^{-1} f \\ &= F^n - f^\dagger \Lambda_+ B_+ L M^{-1} B_- \Lambda_- L^{-1} f. \end{aligned} \quad (2.77)$$

Hence

$$F^n = (U_-^\dagger + g^\dagger)M(U_- + g) + f^\dagger \Lambda_+ B_+ L M^{-1} B_- \Lambda_- L^{-1} f, \quad (2.78)$$

of which the first term is negative definite and the second term is given in terms of f , which is prescribed and can therefore be controlled. Note that homogeneous MDBC give a non-increasing energy while inhomogeneous MDBC give an energy bounded by the free data.

Considering a specific example - continuing with the example of the wave equation - we have the energy density

$$\epsilon = \pi^2 + (\partial_i \phi)^2 \quad (2.79)$$

and the flux

$$F_i = 2\pi \partial_i \phi \quad (2.80)$$

and the flux in the normal direction in terms of the characteristic variables

$$F_n = \frac{1}{4}(U_+^2 - U_-^2), \quad (2.81)$$

where the characteristic variables are no longer vectors. With homogeneous boundary conditions, i.e. with f set to zero, (2.81) becomes

$$F^n = (\kappa^2 - 1)U_-^2, \quad (2.82)$$

showing that F^n is non-positive for $|\kappa_i| \leq 1$. This implies that the time derivative of the energy is non-positive for $|\kappa_i| \leq 1$ and hence the energy cannot grow.

For the case where $f \neq 0$, we don't get a conserved energy but we do get a bound on the energy dependent only upon κ and f . We have to make the condition that $|\kappa| \neq 1$ so we are excluding Dirichlet and Neumann boundary conditions.

$$F^n = \frac{1}{2}(\kappa^2 - 1) \left(U_- + \frac{\kappa f}{\kappa^2 - 1} \right)^2 - \frac{1}{2} \frac{f^2}{\kappa^2 - 1}, \quad (2.83)$$

where the first term is negative and the second is positive but is dependent only upon f and κ and will therefore give a bound on the growth of the energy due to (2.68).

2.6 Constraint preserving boundary conditions

Constraint preserving boundary conditions work in the same way as homogeneous maximally dissipative boundary conditions but instead of controlling the

main energy, they ensure that the constraint energy is non-increasing. To calculate a constraint energy, the constraint system is written in closed form and the constraint characteristic variables are calculated for this system, allowing the constraint energy to be constructed from characteristic constraint variables in the same way as the main energy is constructed from the characteristic variables of the main system.

For the formulations we are considering in this work

$$C_{\pm} = \partial_n U_{\pm} + \dots, \quad (2.84)$$

where the dots stand for transverse derivatives of characteristic variables and where C_{\pm} are a pair of constraint characteristic variables corresponding to the characteristic variables with evolution equations

$$\dot{U}_{\pm} = \pm \partial_n U_{\pm} + \dots \quad (2.85)$$

For example, with KWB (see Section 6.2)

$$C_{\pm} = \partial_n U_{\pm} + \partial^B U_{\pm B}. \quad (2.86)$$

To obtain a constraint energy that is non-growing, homogeneous maximally dissipative boundary conditions can be applied to pairs of characteristic constraint variables.

$$C_+ = \kappa C_-, \quad (2.87)$$

where $|\kappa| \leq 1$. Now substituting (2.84) into this boundary condition gives

$$\partial_n U_+ - \kappa \partial_n U_- = \dots \quad (2.88)$$

This can be translated into an evolution equation using (2.85)

$$\partial_t U_+ + \kappa \partial_t U_- = \dots \quad (2.89)$$

A new variable X on the boundary can be defined as

$$X \equiv U_+ + \kappa U_- \quad (2.90)$$

and therefore (2.89) can be written as

$$\partial_t X = \dots \quad (2.91)$$

This can be viewed as an evolution equation for X on the boundary. X will therefore be known on the boundary and can be used as a source function for a maximally dissipative boundary condition

$$U_+ = -\kappa U_- + X. \quad (2.92)$$

Considering a single pair of characteristic variables, the time derivative of the energy can therefore be bounded by X , as with maximally dissipative boundary conditions, i.e. (2.78) with $M = \kappa^2 - 1$, $L = \kappa$, $\Lambda_+ B_+ = 1$ and $\Lambda_- B_- = -1$.

$$\begin{aligned} \dot{E} &\leq \int_{\partial\Omega} \frac{1}{1 - \kappa^2} X^2 ds \\ &= K_3 \|X\|_{\partial\Omega}^2, \end{aligned} \tag{2.93}$$

where $K_3 = 1/(1 - \kappa^2)$ provided $|\kappa| \neq 1$. Hence the energy is bounded if X is bounded, giving a bound on the solution u . However, bounding X is not easy to do. This can be done if X decouples from the solution in the bulk, i.e. the time derivative can be written in terms of the free boundary data and X itself. However, this is not the case for our work and so we will not be able to prove stability in this way.

Chapter 3

Finite Differencing

3.1 Discrete stability and convergence

Once the continuum problem has been shown to be well-posed, we discretise the equations using difference operators to approximate derivatives. To translate to a full discrete system involves writing complicated discretisations in space and time of the continuum derivatives. However, we use the ‘method of lines’ technique to simplify the problem. This involves considering the semidiscrete problem, i.e. discretising the spatial derivatives but keeping the time derivative continuous, to give a system of ODE’s. For example, the wave equation at the continuum is

$$\dot{\pi} = \psi' \tag{3.1}$$

$$\dot{\psi} = \pi', \tag{3.2}$$

for which we can write the standard second order accurate centred approximation for a first derivative:

$$D_0 u_i = \frac{u_{i+1} - u_{i-1}}{2h}, \tag{3.3}$$

where u_j is the value of u at grid point j and h is the grid spacing, to give

$$\dot{\pi} = \frac{\psi_{i+1} - \psi_{i-1}}{2h} \tag{3.4}$$

$$\dot{\psi} = \frac{\pi_{i+1} - \pi_{i-1}}{2h}. \tag{3.5}$$

These can then be integrated by a standard time-integrator (we will be using 4th order Runge Kutta) as we now have two ODE’s.

We need the discretized solution to converge to the exact solution, i.e. the norm of the error between the numerical and exact solutions must tend to zero as

the time and spatial steps tend to zero, as we need to be able to get closer to the continuum solution by increasing resolution. As a simpler way of showing convergence of a numerical scheme, we can use the Lax theorem, which states that if a numerical scheme is consistent with a well-posed initial value problem in a certain norm and stable with respect to the same norm then it is convergent to the same order and with respect to that norm.[8] Consistency means that a numerical scheme is a good approximation to a problem, i.e. if you substitute the solution of the partial differential equation into the finite difference scheme, you should get an error $\Delta t \tau^n$ where $\|\tau^n\| \rightarrow 0$ as the time and spatial steps tend to zero. Generally we will be specifying operators that are of the correct accuracy so this condition will automatically be satisfied. The problem we will consider more will be that of stability, which means we can bound the solution at time t , i.e. we can put the estimate $\|u^n\| \leq K e^{\alpha t} \|u^0\|$ on the norm of the solution, $\|u^n\|$, where $\|u^0\|$ is the norm of the initial data. Note that the exponential term in this definition of stability allows the solutions of differing initial data to grow apart at a large rate, however it is sufficient for convergence. There is a distinction between this unwanted growth of the solution and a technical numerical instability. The former means that you can always get nearer to the continuum solution simply by increasing the resolution of your scheme while the latter does not allow this.

3.2 Semi-discrete boundaries

Above we gave the maximally dissipative boundary conditions at the continuum level. However, when forming the discrete numerical scheme, specifying the semi-discrete system for the points on the boundary will usually require spatial differences. In the bulk a centered difference operator is often used but on the boundary, some prescription using one-sided difference operators is needed. For example, considering a one-dimensional grid, where the first grid point is $j = 0$ and the last grid point is $j = N$ we may need operators like the first order approximations of the first spatial derivatives:

$$D_+ u_0 = \frac{u_1 - u_0}{h} \quad (3.6)$$

and

$$D_- u_N = \frac{u_N - u_{N-1}}{h}, \quad (3.7)$$

as we cannot use points from outside the grid. That is, unless we make use of ghost-points, which are points outside the physical grid that can be used in the

same centered derivative operators at the boundary as in the bulk of the grid. So in general, the continuum boundary conditions need to be translated into one-sided derivative operators (making use of the semidiscrete evolution equations in the calculation) or they need to be used to populate these ghost-points. These techniques are equivalent, however it turns out that the second method is easier for coding purposes whilst the first is more suited to analysis.

Considering the maximally dissipative boundary conditions described above, we can use the wave equation as an example of forming a semi-discrete prescription.

3.2.1 The second order in space wave equation

Here we will consider the wave equation in second order in space form in only one dimension for simplicity.

$$\dot{\phi} = \pi, \quad (3.8)$$

$$\dot{\pi} = \phi'', \quad (3.9)$$

which we discretise with

$$\dot{\phi}_j = \pi_j \quad (3.10)$$

$$\dot{\pi}_j = D_+ D_- \phi_j, \quad (3.11)$$

where the subscript denotes the grid location. As calculated above, the characteristic variables are

$$U_{\pm} = \pi \pm \phi', \quad (3.12)$$

with evolution equations

$$\dot{U}_{\pm} = \pm U'_{\pm}. \quad (3.13)$$

Again, we consider a 1D grid from $j = 0$ to $j = N$ (parameters subscripted with L and R represent the values on the left and right boundaries respectively).

At the boundary of the grid, $j = N$

$$U_+ \doteq \kappa U_- + f \quad |\kappa| < 1, \quad (3.14)$$

where $|\kappa|$ is set to be strictly less than one so we avoid any problem with equation (2.83).

Substituting the evolution variables back into (3.14) gives

$$\phi'_N \doteq - \frac{\pi_N(\kappa_R - 1) - f_R}{\kappa_R + 1}. \quad (3.15)$$

We discretise the first derivative with a second order accurate difference operator

$$D_0 u_N = \frac{u_{N+1} - u_{N-1}}{2h} \quad (3.16)$$

and make use of the fact that

$$D_+ D_- = \frac{2}{h}(D_0 - D_-) = \frac{2}{h}(D_+ - D_0) \quad (3.17)$$

to give the second order accurate spatial discretisation. The semi-discrete evolution of the system on the boundary is therefore

$$\dot{\phi}_N \doteq \pi_N \quad (3.18)$$

$$\dot{\pi}_N \doteq \frac{2}{h} \left(-D_- \phi_N - \pi_N \frac{\kappa_R - 1}{\kappa_R + 1} + \frac{f_R}{\kappa_R + 1} \right). \quad (3.19)$$

Chapter 4

3+1 Formulations of General Relativity

4.1 The 3+1 split

There are various approaches for breaking down the Einstein equations; the two most common are the 3+1 split and the characteristic 2+2 split. We will concentrate on the former as it allows us to give data on an initial spatial hypersurface and make a discrete evolution of data onto subsequent hypersurfaces, using a time vector. In the following calculation we follow closely the work of York.[9]

The first task is to foliate the spacetime with 3-surfaces. We can prescribe a unit normal, n_i , to the 3-surfaces that can be used to form the spatial metric on the slices:

$$\gamma_{ab} = g_{ab} + n_a n_b, \quad (4.1)$$

where g_{ab} is the 4D metric. Contracting with n^a and making use of $n^a n_a = -1$ gives

$$\gamma_{ab} n^a = 0, \quad (4.2)$$

showing that the 3D metric is perpendicular to the normal. It should be noted that the mixed form of the 3-metric $\perp_b^a = \gamma_b^a = \delta_b^a + n^a n_b$ is a projector onto the slices,

$$\perp_c^a \perp_b^c = (\delta_c^a + n^a n_c)(\delta_b^c + n^c n_b) = \delta_b^a + n^a n_b = \perp_b^a. \quad (4.3)$$

The projection operator can be used to project the 4D covariant derivative ∇ onto

the slices to give the 3D covariant derivative D .

$$D_a w^b \equiv \perp \nabla_a w^b \equiv \perp_a^c \perp_d^b \nabla_c w^d. \quad (4.4)$$

Now

$$\nabla_a g_{bc} = 0. \quad (4.5)$$

In analogy to (4.5) the 3D covariant derivative of the spatial metric, $D_a \gamma_{bc}$, vanishes:

$$\begin{aligned} D_a \gamma_{bc} &= \perp_a^d \perp_b^e \perp_c^f \nabla_d \gamma_{ef} \\ &= \perp_a^d \perp_b^e \perp_c^f \nabla_d g_{ef} + n_e \perp_a^d \perp_b^e \perp_c^f \nabla_d n_f + n_f \perp_a^d \perp_b^e \perp_c^f \nabla_d n_e \\ &= 0, \end{aligned} \quad (4.6)$$

where we have expanded the projector, used the linearity and Leibniz rules and eliminated any terms of the form $\nabla_a g_{bc} = 0$ and $\perp_a^b n_b = 0$.

We have a metric and a covariant derivative for the 3-surfaces; all that remains to give a full description of the spacetime is to define how the surfaces are embedded in the manifold. This description is contained within the term known as the extrinsic curvature K_{ab} , which can be considered to be the time derivative of the 3-metric. It incorporates the information difference between the 4D Riemann tensor and the 3D Riemann tensor. We have the four main definitions of K_{ab} (the proof that they are equivalent can be found in Appendix A).

$$K_{ab} = -\frac{1}{2} \perp \mathcal{L}_n g_{ab} \quad (4.7)$$

$$= \perp \nabla_{(a} n_{b)} \quad (4.8)$$

$$= -\frac{1}{2} \mathcal{L}_n \gamma_{ab} \quad (4.9)$$

$$= -\nabla_a n_b - n_a a_b, \quad (a_b = n^c \nabla_c n_b), \quad (4.10)$$

where $\mathcal{L}_c T_{ab} = n^c \partial_c T_{ab} + T_{cb} \partial_a n^c + T_{ac} \partial_b n^c$ and \perp projects each of the indices.

We can define a time vector t^a as threading the 3-surfaces, in the same direction as n^a , mapping points on one spatial hypersurface, say Σ_t , to points on the next hypersurface, say $\Sigma_{t+\Delta t}$ (see figure 4.1). This time vector can be constructed from a multiple of the normal n^a , where this multiple is called the lapse α , and the shift β , which describes the movement of the points in space between the two hypersurfaces. Hence, we can write the time vector explicitly as

$$t^a = \alpha n^a + \beta^a. \quad (4.11)$$

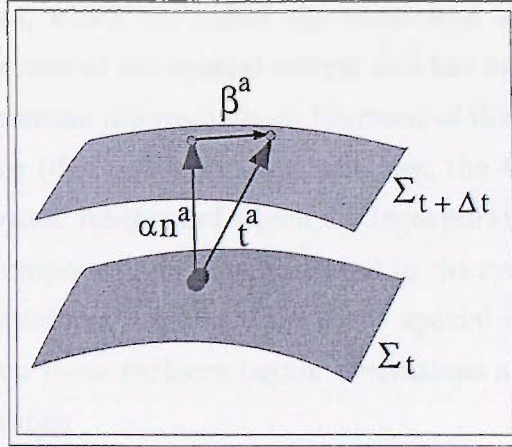


Figure 4.1: Spatial hypersurfaces threaded by the unit normal and the time vector (one dimension suppressed).

We can now define the 3D Riemann tensor in an analogous way to its 4D counterpart by writing:

$$D_{[a}D_{b]}w_c = \frac{1}{2}R^d{}_{cba}w_d \quad (4.12)$$

and

$$R^d{}_{cba}n_d = 0, \quad (4.13)$$

the latter coming from the fact that the 3D Riemann tensor must be spatial. The Gauss equation below expresses the 4D Riemann tensor in terms of the 3D Riemann tensor and the extrinsic curvature. It involves a projection of all four indices of the 4D Riemann tensor.

$${}^{(3)}R_{abcd} = \perp^{(4)}R_{abcd} + K_{ad}K_{bc} - K_{ac}K_{bd}. \quad (4.14)$$

The derivations of this and the following equations can be found in Appendix A. The Codazzi equation involves a projection of three indices onto the spatial slices and a contraction with the unit normal.

$$D_b K_{ac} - D_a K_{bc} = \perp R_{abcn}, \quad (4.15)$$

where $R_{abcn} = n^d R_{abcd}$.

The one remaining decomposition requires two projections and two contractions with the normal, which will give the evolution equations, i.e. the time derivatives of the extrinsic curvature and the spatial metric. This is in contrast to the Gauss and Codazzi equations, which are called the constraint equations because they involve no time derivatives of the spatial metric and the extrinsic curvature. The constraint equations contain information on fourteen of the twenty components of the 4D Riemann tensor (due to symmetry properties, the 4D Riemann tensor has twenty degrees of freedom, fourteen of which are incorporated in these equations). Hence, the other six components are incorporated in the evolution equations. The Gauss and Codazzi equations must hold for every spatial slice and so give rise to constraint equations on these surfaces (again derivations are in Appendix A). Of the ten Einstein equations

$$G_{ab} = 8\pi T_{ab}, \quad (4.16)$$

one becomes the scalar or Hamiltonian constraint

$$2G_{nn} = R + K^2 - K_{ab}K^{ab} = 16\pi\rho, \quad (4.17)$$

where $\rho = T_{nn}$, and three become the momentum constraint

$$G^{an} = D_b(\gamma^{ab}K - K^{ab}) = \kappa j^a, \quad (4.18)$$

where we make a slight change of notation to [9] with $\perp G^{an} \equiv \perp G_n^a$ and $j^a \equiv \perp T^{an}$. The momentum constraint is so named because it involves the momentum density as determined by an observer moving with the slices. The ρ in the Hamiltonian constraint can be viewed as the energy density in a similar way.

In summary, we have the Hamiltonian constraint, which embodies one of the Einstein equations, and the momentum constraint, which incorporates another three. Whereas these four constraints hold on the slices, the remaining six Einstein equations are related to the embedding of the slices in spacetime. Here is where the Lie derivative with respect to $N^a = \alpha n^a$ enters into the calculation. Whilst the constraint equations do not contain any time derivatives of the extrinsic curvature or spatial metric and hence are not involved in the evolution of the solution, the remaining equations give expression for $\mathcal{L}_N K_{ab}$ and $\mathcal{L}_N \gamma_{ab}$ and hence describe evolution between the spatial hypersurfaces.

$$\mathcal{L}_N K_{ab} = -\alpha \perp R_{anbn} + D_a D_b \alpha + \alpha K_{ac} K_b^c. \quad (4.19)$$

This can be translated into the Lie derivative of the curvature in the direction of time by using $\mathcal{L}_t = \mathcal{L}_N + \mathcal{L}_\beta$ and expanding the projections of the Ricci tensor and the contracted Riemann tensor.

$$\begin{aligned} \mathcal{L}_t K_{ab} = & -D_a D_b \alpha + \alpha [R_{ab} - 2K_{ac} K_b^c + K_{ab} K \\ & - \kappa (S_{ab} - \frac{1}{2} \gamma_{ab} S) - \frac{1}{2} \kappa_\rho \gamma_{ab}] + \mathcal{L}_\beta K_{ab}, \end{aligned} \quad (4.20)$$

where we have introduced the projection of the stress-energy tensor onto the slices, S_{ab} . Note that because we are in a coordinate system that is adapted to the vector field t^a , $\mathcal{L}_t = \partial_t$, illustrating why we consider these equations as evolution equations.[10] The evolution equation for the extrinsic curvature (4.20) in addition to the evolution equation for the spatial metric

$$\mathcal{L}_t \gamma_{ab} = -2\alpha K_{ab} + \mathcal{L}_\beta \gamma_{ab}, \quad (4.21)$$

and the momentum and Hamiltonian constraints give the full ten Einstein equations. (4.20) and (4.21) detail how the extrinsic curvature and the metric change with time but they say nothing about the lapse and shift, as these are a gauge choice.

Initial data of the form $(\gamma_{ij}, K_{ij}, \rho, j_i)$ can be specified on a 3D spatial surface. Due to the contracted Bianchi identities,

$$\nabla^a G_{ab} = 0, \quad (4.22)$$

if the initial data satisfies the constraints then the solution will always satisfy the constraints throughout the evolution.[10]

4.2 Adapting the Einstein equations

4.2.1 Evolution of the Einstein equations

As was shown in the previous section, the deconstruction of the Einstein equations into the 3+1 split provides six evolution equations, which involve time derivatives of the 3-metric and the extrinsic curvature, and four constraint equations, which do not involve time derivatives. There are two methods of implementing these equations; ‘constrained’ evolution involves using a mixture of the evolution equations and the constraint equations to solve the field equations whilst ‘free’

evolution solves the constraints on the initial hypersurface and then uses only the evolution equations, leaving the constraint equations to be used as a test on the solution to check how closely it satisfies the constraints. The reason that constrained evolution is largely avoided is the requirement of more processing power, due to the need to solve the elliptic constraint equations, whilst free evolution is more economical on processing time. If the constraints are satisfied initially, then at the continuum they will be satisfied throughout the evolution, so in this case, at the continuum, constrained and free evolution are equivalent. However, free evolution allows constraint violation from numerical error and so the constraints will not remain satisfied at the discrete level. One of the advantages of the presence of constraints in free evolution is that they provide an additional tool for reformulating the evolution equations in addition to the standard change of variables, whether it be by adding multiples of the constraints (in essence adding zero to the continuum equations) or introducing auxiliary variables (which adds new constraints for these new variables.) When the constraints are obeyed, the same equations are being solved at the continuum, however these adjustments can aid stability at the discrete level. It should be noted that this method of using the constraints to obtain well-posedness is distinct from constrained evolution because it involves adding the constraints to the evolution equations, rather than replacing a number of evolution equations with constraint equations, and hence retains the bifurcation into six evolution equations and four constraint equations.

4.2.2 The ADM system

The scheme derived in the previous section was the original formulation used in numerical relativity, called the ADM formulation after Arnowitt, Deser and Misner and introduced to the numerical community by Smarr and York [11] and York.[9] Although this was the standard formulation used in numerical relativity up until the mid 1990's, numerical codes were plagued with unexplained blow-ups, which were thought to be caused by insufficient resolution, a bad choice of gauge or just an unstable finite differencing scheme. However, it was later discovered that the formulation itself was ill-posed at the continuum with certain gauge choices, and numerical error was triggering instabilities.

4.2.3 The BSSN system

Various modifications to the ADM formulation have been suggested and tested over the years. The first to be mentioned here is the BSSN system, introduced by Nakamura and Shibata in 1995 [2] and reintroduced by Baumgarte and Shapiro in 1999 [3], which involves introducing new ‘connection’ variables and factoring out the conformal factor. This means that instead of evolving the extrinsic curvature and the metric, the variables evolved are the conformal factor and the trace of the extrinsic curvature. The new variables are the conformal metric $\tilde{\gamma}_{ij}$, the conformal tracefree part of the extrinsic curvature \tilde{A}_{ij} and the conformal connection variables $\tilde{\Gamma}^i$

$$\tilde{\gamma}_{ij} = e^{-4\phi} \gamma_{ij} \quad (4.23)$$

$$\tilde{A}_{ij} = e^{-4\phi} \left(K_{ij} - \frac{1}{3} \gamma_{ij} K \right) = e^{-4\phi} A_{ij} \quad (4.24)$$

$$\tilde{\Gamma}^i = \tilde{\Gamma}_{jk}^i \tilde{\gamma}^{jk}. \quad (4.25)$$

where $\phi = \frac{1}{12} \log(\det \gamma_{ij})$ is chosen so that the additional constraint $\tilde{\gamma} = \det \tilde{\gamma}_{ij} = 1$ is satisfied. The most essential modification for numerical stability was stated in [3] to be the use of the momentum constraint to eliminate the divergence of \tilde{A}_{ij} .

There are many forms of the BSSN equations that are used by different groups and it is important to note that the hyperbolicity depends very much on how the equations are written. The BSSN system with densitised lapse and fixed shift in [13] is shown to be strongly hyperbolic. Also, in [12] a general form of BSSN is shown with conditions on the parametrisation of the addition of constraints that give strong hyperbolicity.

4.2.4 The NOR system

An alternative is the NOR formulation, introduced by Nagy, Ortiz and Reula [1] and derived from the densitised ADM system in a similar way to BSSN (but without a conformal traceless decomposition) by introducing three connection variables, similar to the Γ^i variables in BSSN, and adding a multiple of the momentum constraint to the evolution equation of f_i . The evolution equations are

$$\mathcal{L}_{(t-\beta)} \gamma_{ij} = 2NK_{ij} \quad (4.26)$$

$$\mathcal{L}_{(t-\beta)} K_{ij} = \frac{N}{2} \gamma^{kl} [-\gamma_{ij,kl} - b\gamma_{kl,ij}] + Nf_{(j,i)} + \mathcal{B} \quad (4.27)$$

$$\mathcal{L}_{(t-\beta)} f_i = N[(c-2)\gamma^{kj} K_{ij,k} + (1-c)\gamma^{kj} K_{kj,i}] + \mathcal{C}_i \quad (4.28)$$

and the constraints are

$${}^{(3)}R + K^2 - K_{ab}K^{ab} = 2\kappa\rho \quad (4.29)$$

$$D_b K_a^b - D_a K = \kappa\rho \quad (4.30)$$

$$f^\mu - \gamma^{\nu\sigma}\gamma_{\nu\sigma}^\mu = 0. \quad (4.31)$$

Note we have used γ_{ij} here instead of h_{ij} to keep notation consistent.

If the f^i are introduced as in [12] with arbitrary $\rho = r + 2$ (instead of $\rho = 1$ in [1]), then the equations with zero shift and densitised lapse linearised about Minkowski space can be written as in [6] with $b = 1$, $c = 2$ in the notation of [1]

$$\partial_t \gamma_{ij} = -2K_{ij} \quad (4.32)$$

$$\partial_t K_{ij} = -\frac{1}{2}\partial^k \partial_k \gamma_{ij} + \frac{r}{2}\partial_i \partial_j t + \partial_{(i} f_{j)} \quad (4.33)$$

$$\partial_t f_i = r\partial_i K, \quad (4.34)$$

where $t = \delta^{kl}\gamma_{kl}$. This form is how we will compare to the electromagnetic formulations we consider later.

It was shown in [1] that the pseudo-differential reduction of NOR is strongly hyperbolic for (i) $b > 0$, $b \neq 1$ and $c > 0$ and (ii) $b = 1$ and $c = 2$, and hence for the case in [6].

4.2.5 The Z4 system

Another technique is to introduce extra variables into the field equations before the 3+1 split is made. An example of this is the Z4 system where the auxiliary variable Z_μ is introduced into the Einstein equations in the following way

$$R_{\mu\nu} + \nabla_\mu Z_\nu + \nabla_\nu Z_\mu = 8\pi(T_{\mu\nu} - \frac{1}{2}Tg_{\mu\nu}), \quad (4.35)$$

where setting $Z_\mu = 0$ regains the Einstein equations. By splitting up the auxiliary variable into the spatial component Z_i and the normal component $\Theta \equiv -n_\mu Z^\mu = \alpha Z^0$ (where n_μ is the unit normal to the slices), the 3+1 decomposition in vacuum can be made:[4]

$$(\partial_t - \mathcal{L}_\beta)\gamma_{ij} = -2\alpha K_{ij} \quad (4.36)$$

$$\begin{aligned} (\partial_t - \mathcal{L}_\beta)K_{ij} &= -D_i D_j \alpha + \alpha[R_{ij} + D_i Z_j + D_j Z_i \\ &\quad - 2K_{ik}K^k_j + (K - 2\theta)K_{ij}] \end{aligned} \quad (4.37)$$

$$(\partial_t - \mathcal{L}_\beta)\theta = \frac{\alpha}{2}[R + (K - 2\theta)K - K^{ij}K_{ij} + 2D_k Z^k - 2(D_k \alpha / \alpha)Z^k] \quad (4.38)$$

$$(\partial_t - \mathcal{L}_\beta)Z_i = \alpha[D_k(K_i^k - \delta_i^k K) + D_i \Theta - (D_i \alpha / \alpha)\Theta - 2K_i^k Z_k], \quad (4.39)$$

with the usual constraints

$$H \equiv R - K_{ij}K^{ij} + K^2 \quad (4.40)$$

$$M_i \equiv D^j K_{ji} - D_i K. \quad (4.41)$$

Note that the constraint equations that existed before the introduction of the auxiliary variable have been translated into evolution equations for that variable. For a solution of the Einstein equations, the Hamiltonian and momentum constraints must be satisfied for the initial data as well as setting $Z_\mu = 0$. It is important to notice that the constraint system only closes if equations (4.38) and (4.39) are included and hence the variable Z_μ is a part of the constraint system and the evolution system, a fact that is useful when trying to damp constraints; by controlling Z_μ in the evolution equations, we can damp the constraints without having to project back onto the constraint surface. The variable Z_μ can be used in a breaking of the time symmetry, which allows damping of the constraint and hence produces an attracting constraint hypersurface. A damping parameter κ is added into the field equations [14]:

$$R_{\mu\nu} + D_\mu Z_\nu + D_\nu Z_\mu - \kappa[t_\mu Z_\nu + t_\nu Z_\mu - g_{\mu\nu}t^\lambda Z_\lambda] = 0, \quad (4.42)$$

where t^μ is a time-like vector. This introduces extra terms involving κ into (4.37), (4.38) and (4.39) and the damping of constraints described above.

We also note from [14] that the transformation

$$\Theta \rightarrow 0, \quad Z_i \rightarrow \frac{1}{2} \left(f_i - \gamma^{jk} \gamma_{ij,k} + \frac{\rho}{2} \gamma^{jk} \gamma_{jk,i} \right) \quad (4.43)$$

takes the Z4 system to NOR.

Chapter 5

Electromagnetism

5.1 Electromagnetic analogues of formulations of general relativity

Some formulations of the Einstein equations have an electromagnetic analogue, including the Z4 and NOR systems mentioned above. The advantage of working with these analogues is that electromagnetism is linear rather than quasi-linear (linear in the highest derivatives) and exact solutions can be given to compare to the results of a numerical scheme, allowing simple convergence tests.

5.2 The Maxwell equations

To make a 3+1 split of the Maxwell equations we can start from the field equations (the derivation from the differential form of the Maxwell equations can be found in Appendix B):

$$F^{\mu\nu}{}_{,\mu} = -4\pi j^\nu \quad (5.1)$$

$$F_{\mu\nu} \equiv A_{\nu,\mu} - A_{\mu,\nu}, \quad (5.2)$$

with the conservation of charge

$$j^\mu{}_{,\mu} = 0. \quad (5.3)$$

We define $A^0 \equiv \psi$, $j^0 \equiv \rho$ and the electric field $E_i \equiv F_{i0} = -\dot{A}_i + \psi_{,i}$ from equation (5.2). Setting $\nu = 0$ in 5.1 gives $E_{i,i} = 4\pi\rho$ whilst setting $\nu = i$ gives

$\dot{E}_i = -(A_{i,jj} - A_j, ij) - 4\pi j_i$, and we can therefore write out the full system:

$$\dot{A}_i = -E_i - \psi_{,i} \quad (5.4)$$

$$\dot{E}_i = A_{j,ji} - A_{i,jj} - 4\pi j_i \quad (5.5)$$

$$0 = C \equiv E_{i,i} - 4\pi \rho. \quad (5.6)$$

E_i is the electric field, A_i is the magnetic potential, ψ is the electric potential and j_i and ρ are source terms that satisfy $j_i^i + \dot{\rho} = 0$. For simplicity, the vacuum case ($\rho = j_i = 0$) will be considered with the electric potential ψ also set to zero. In a comparison to the ADM equations, A_i can be considered analogous to the spatial metric γ_{ij} , E_i to the extrinsic curvature K_{ij} and the constraint C to the ADM momentum constraint.

Next, we make a differential reduction to first order by introducing new variables for the first derivatives of the magnetic potential. The new variable d_{ij} is defined as

$$d_{ij} = \partial_i A_j \quad (5.7)$$

and the fact that $\partial_i \partial_j A_k$ can be written as $\partial_j d_{ik}$ or $\partial_i d_{jk}$ gives rise to an additional constraint.

$$0 = C_{ijk} \equiv \partial_i d_{jk} - \partial_j d_{ik}. \quad (5.8)$$

The original system of equations is rewritten as

$$\dot{A}_i = -E_i \quad (5.9)$$

$$\dot{E}_i = c \partial_i d_{jj} + (1 - c) \partial_j d_{ij} - \partial_j d_{ji} \quad (5.10)$$

and differentiating (5.9) gives

$$\partial_j \dot{A}_i = -\partial_j E_i. \quad (5.11)$$

The evolution equations are therefore

$$\dot{E}_i = c \partial_i d_{jj} + (1 - c) \partial_j d_{ij} - \partial_j d_{ji} \quad (5.12)$$

$$\dot{d}_{ij} = -\partial_i E_j, \quad (5.13)$$

which with the constraints

$$0 = C_{ijk} \equiv \partial_i d_{jk} - \partial_j d_{ik} \quad (5.14)$$

$$0 = C \equiv \partial_i E_i \quad (5.15)$$

provide the full system in first order form, where the evolution equations can be written in the standard way

$$\partial_t \mathbf{u} = P^i \partial_i \mathbf{u}. \quad (5.16)$$

For arbitrary direction n_i , a strongly hyperbolic system is one where the matrix $P_n = n_i P^i$ has only real eigenvalues and a complete set of eigenvectors. A projector onto the space normal to n_i can be given as usual

$$q^i_j \equiv \delta^i_j - n^i n_j, \quad (5.17)$$

where a projected index is denoted by A, B, C . So

$$\partial_t \mathbf{u} = P_n \partial_n \mathbf{u} + P^A \partial_A \mathbf{u}. \quad (5.18)$$

Considering the example $n = (1, 0, 0)$,

$$q^{ij} = \delta^{ij} - \delta_1^i \delta^{1j} \quad (5.19)$$

and the variable d_{ij} can be broken down into a scalar block

$$d_{nn} = d_{11} \quad (5.20)$$

$$\begin{aligned} d_{qq} &\equiv d_{ij} q^{ij} = (d_{11} + d_{22} + d_{33}) - d_{11} \\ &= d_{22} + d_{33}, \end{aligned} \quad (5.21)$$

the transverse vector block

$$d_{nA} = (d_{12}, d_{13}) \quad (5.22)$$

$$d_{An} = (d_{21}, d_{31}) \quad (5.23)$$

and the transverse traceless tensor block

$$d_{AB} = \begin{pmatrix} \frac{1}{2}(d_{22} - d_{33}) & d_{23} \\ d_{32} & \frac{1}{2}(d_{33} - d_{22}) \end{pmatrix}.$$

Therefore, returning to n, A notation, the evolution equations of the components of d_{ij} are

$$\partial_t d_{nn} = -\partial_1 E_1 \quad (5.24)$$

$$\partial_t d_{nA} = -\partial_1 E_A \quad (5.25)$$

$$\partial_t d_{An} = -\partial_A E_1 \quad (5.26)$$

$$\partial_t d_{AB} = -\partial_A E_B \quad (5.27)$$

$$\partial_t d_{qq} = -\partial_A E_A. \quad (5.28)$$

The remaining evolution equations are

$$\begin{aligned}\partial_t E_n &= -\partial_n d_{nn} - \partial_A d_{An} + c\partial_n d_{nn} + c\partial_n d_{qq} + (1-c)\partial_n d_{nn} + (1-c)\partial_A d_{nA} \\ &= -\partial_A d_{An} + c\partial_n d_{qq} + (1-c)\partial_A d_{nA}\end{aligned}\quad (5.29)$$

$$\partial_t E_A = -\partial_n d_{nA} - \partial_B d_{BA} + c\partial_A d_{nn} + c\partial_A d_{BB} + (1-c)\partial_n d_{An} + (1-c)\partial_B d_{AB}.\quad (5.30)$$

Ignoring transverse derivatives we can write down P_n . However, the variables split into scalar, vector and tensor blocks and can be considered separately. For the scalar block: (d_{nn}, E_n, d_{qq}) ,

$$P^n = \begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & c \\ 0 & 0 & 0 \end{pmatrix},$$

for which the only eigenvalue is $\lambda = 0$ with only one eigenvector $(1, 0, 0)$. There is not a full set of eigenvectors and the system is therefore only weakly hyperbolic. To be strongly hyperbolic, for any n , P_n has to have real eigenvalues and a complete set of eigenvectors. For the transverse vector block, (d_{nA}, E_A, d_{An}) ,

$$P^n = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & (1-c) \\ 0 & 0 & 0 \end{pmatrix}$$

has eigenvalues $\lambda = 0, \pm 1$ and eigenvectors $(1-c, 0, 1)$ and $(-1, \pm 1, 0)$. The transverse traceless tensor block d_{AB} has $P_n = 0$.

5.3 The KWB system

The KWB system can be obtained from equations (5.4 - 5.6) by introducing the variable

$$\Gamma = \partial_j A_j, \quad (5.31)$$

which gives rise to an additional constraint

$$0 = C_\Gamma \equiv \Gamma - \partial_j A_j. \quad (5.32)$$

The constraints can then be used to give the time derivative for Γ

$$\dot{\Gamma} = \partial_j \dot{A}_j = -\partial_j E_j = 0 \quad (5.33)$$

from the constraint

$$0 = C \equiv \partial_j E_j. \quad (5.34)$$

This alters the system of equations to

$$\dot{A}_i = -E_i \quad (5.35)$$

$$\dot{E}_i = -\partial^j \partial_j A_i + \partial_i \Gamma \quad (5.36)$$

$$\dot{\Gamma} = 0, \quad (5.37)$$

with constraints

$$0 = C \equiv \partial_j E_j \quad (5.38)$$

$$0 = C_\Gamma \equiv \Gamma - \partial_j A_j. \quad (5.39)$$

This is the simplest form of the general set of equations

$$\dot{A}_i = -E_i \quad (5.40)$$

$$\dot{E}_i = -\partial^j \partial_j A_i + (1 - a)\partial^j \partial_i A_j + a\partial_i \Gamma \quad (5.41)$$

$$\dot{\Gamma} = (1 - b)\partial_j E_j, \quad (5.42)$$

with a and b set to 1.[15]

The analogy between NOR and KWB can be made clear by comparing the 3-metric γ_{ij} with A_i , the extrinsic curvature K_{ij} with E_i and the auxiliary connection variables f_i with Γ . Note, the construction of KWB parallels that of NOR in that the new variable Γ is introduced in the same way as f_i and the constraint is added to an evolution equation to make the formulation strongly hyperbolic. The analogy cannot be taken too far however because the Γ variable decouples from the evolution equations in KWB, a property that does not hold for the f_i terms in NOR; considering equation (4.28), γ_{ij} and K_{ij} both appear in the evolution equation for f_i .

The characteristic variables of the KWB system can be calculated by first making a first order reduction,

$$\dot{d}_{ij} = -\partial_i E_j \quad (5.43)$$

$$\dot{E}_i = -\partial_j d_{ji} + \partial_i \Gamma \quad (5.44)$$

$$\dot{\Gamma} = 0, \quad (5.45)$$

with constraint equations

$$0 = C \equiv \partial^j E_j \quad (5.46)$$

$$0 = C_\Gamma \equiv \Gamma - \partial^j A_j. \quad (5.47)$$

The principal matrix for the scalar block: $(d_{nn}, E_n, d_{qq}, \Gamma)$ is

$$P_n = \begin{pmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

for which the eigenvalues are $\lambda = 0, \pm 1$ and the corresponding eigenvectors are $(1, 0, 0, 1)$, $(0, 0, 1, 0)$ and $(-1, \pm 1, 0, 1)$. The vector block: (d_{nB}, E_B, d_{Bn}) has principal matrix

$$P_n = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

and hence has eigenvalues $\lambda = 0, \pm 1$ and eigenvectors $(0, 0, 1)$ and $(-1, \pm 1, 0)$. We can take the inverse of the matrix of eigenvectors or use the transpose of the principal matrix - recall equation (2.55) - to give the non-zero speed characteristic variables:

$$U_{\pm} = -d_{nn} \pm E_n + \Gamma \quad (5.48)$$

$$U_{\pm B} = -d_{nB} \pm E_B, \quad (5.49)$$

$$(5.50)$$

which in second order form are

$$U_{\pm} = -A_{n,n} \pm E_n + \Gamma \quad (5.51)$$

$$U_{\pm B} = -A_{B,n} \pm E_B. \quad (5.52)$$

The calculation is exactly the same in second order form if $A_{n,n}$ and $A_{B,n}$ are considered as evolution variables.

Considering a domain periodic in x, y and z , the general conserved energy density is

$$2\epsilon = [c_0(E_i^2 + A_{i,j}^2 - 2A_{i,i}\Gamma) + c_1\Gamma^2 + c_2(A_{i,i}^2 - A_{i,j}A_{j,i})]. \quad (5.53)$$

For simplicity, c_0 is set to 1, c_2 is set to 0 and $c_1 = \sigma$ is large enough to ensure that the energy is positive definite. This gives the energy density

$$2\epsilon = E_i^2 + A_{i,j}^2 - 2A_{i,i}\Gamma + \sigma\Gamma^2. \quad (5.54)$$

This energy can be shown to be conserved by taking the time derivative

$$\dot{\epsilon} = (-E_i A_{i,jj} + E_i \Gamma_{,i} - E_{i,j} A_{i,j} + E_{i,i} \Gamma) \quad (5.55)$$

and then the integral over space, where Ω is the domain of the solution,

$$\begin{aligned}\dot{E} &= \int_{\Omega} -E_i A_{i,jj} + E_i \Gamma_{,i} - E_{i,j} A_{i,j} + E_{i,i} \Gamma dV \\ &= \int_{\Omega} (-E_i A_{i,j} + E_j \Gamma)_{,j} dV,\end{aligned}\quad (5.56)$$

which, as we are taking an integral of a total divergence with periodic boundaries, gives a conserved energy by Gauss' Theorem.

To show that the energy is positive definite, $A_{i,j}$ is split into trace and traceless parts: $A_{i,j} = \frac{1}{3} \delta_{ij} S_{kk} + \tilde{S}_{ij}$ so that

$$\begin{aligned}\epsilon &= E_i E^i + \left(\frac{1}{3} \delta_{ij} S_{kk} + \tilde{S}_{ij}\right) \left(\frac{1}{3} \delta^{ij} S_{ll} + \tilde{S}^{ij}\right) - 2S_{kk} \Gamma + \sigma \Gamma^2 \\ &= E_i E^i + \frac{1}{3} (S_{kk})^2 + \tilde{S}_{ij} \tilde{S}^{ij} - 2S_{kk} \Gamma + \sigma \Gamma^2 \\ &= E_i E^i + \frac{1}{3} [S_{kk} - 3\Gamma]^2 + (\sigma - 3)\Gamma^2 + \tilde{S}_{ij} \tilde{S}^{ij},\end{aligned}\quad (5.57)$$

from which it is clear that with $\sigma \geq 3$, the energy is positive definite in E_i , Γ and the first derivative of A_i . The situation when including A_i is a little more complicated, as the energy is no longer conserved, but is instead bounded by exponential growth (see section 6.1.3).

Now, considering a boundary $\partial\Omega$ to the domain Ω , there will be a non-vanishing term

$$\begin{aligned}\dot{E} &= \int_{\partial\Omega} (-E_i A_{i,n} + E_n \Gamma) ds \\ &= \int_{\partial\Omega} (E_n (-A_{n,n} + \Gamma) + E_B (-A_{B,n})) ds\end{aligned}\quad (5.58)$$

$$= \frac{1}{4} \int_{\partial\Omega} ((U_{+i}^2 - U_{-i}^2)) ds.\quad (5.59)$$

The maximally dissipative boundary conditions are

$$U_{+i} = \kappa U_{-i} + f_i.\quad (5.60)$$

With homogeneous MDBC

$$\dot{E} = \frac{1}{4} \int_{\partial\Omega} ((\kappa^2 - 1) U_{-i}^2) ds,\quad (5.61)$$

which is non-increasing for $|\kappa| < 1$. Here, $|\kappa| = 1$ would give a conserved energy. By adding in the inhomogeneous terms the energy will no longer be non-increasing but it will instead be possible to bound it in terms of the inhomogeneous free data.

$$\dot{E} = \frac{1}{4} (\kappa^2 - 1) \left(U_- + \frac{\kappa f}{\kappa^2 - 1} \right)^2 - \frac{1}{2} \frac{f^2}{\kappa^2 - 1}.\quad (5.62)$$

Note, we have given κ no subscript here but in general each MDBC will have a distinct κ_i .

5.4 The Z1 system

An electromagnetic analogue to the Z4 formulation is the Z1 system. The variable Z can be introduced into the Maxwell field equations in the same way as Z_μ was introduced into the field equations for the Z4 system and again it can be set up to damp the constraints.

$$F^{\mu\nu}{}_{,\mu} - Z^{,\nu} - \kappa t^\nu Z = -4\pi j^\nu, \quad (5.63)$$

where $t^\nu = (1, 0, 0, 0)$ and $\kappa \geq 0$ is a damping parameter. The evolution equations can be constructed as above but with the extra terms incorporated.

$$\dot{A}_i = -E_i + \partial_i \psi, \quad (5.64)$$

$$\dot{E}_i = -\partial_j \partial^j A_i + \partial^j \partial_i A_j + \partial_i Z - 4\pi j_i, \quad (5.65)$$

$$\dot{Z} = -\kappa Z + \partial^i E_i - 4\pi \rho. \quad (5.66)$$

Also notice that setting $\Gamma = Z + A_{i,i}$ transforms the KWB system into the undamped Z1 system. It is important to note that the linearised NOR system given above, equations (4.32 - 4.34), can be compared to KWB directly only if the parameter r is set to zero. By a different choice of parameter, the system is equivalent to linearised Z4.

Again, the source terms ρ and j_i are set to zero to study the homogeneous problem and the electric potential ψ is set to zero as a gauge choice. It should be noted that the solution to these equations is a solution of the Maxwell equations only if the constraints $C = E_{i,i}$ and Z are equal to zero. The constraint C has now become an evolution equation for Z in exactly the same way as the constraints become evolution equations for Z_μ in the Z4 system.

For the first order reduction, the auxiliary variable d_{ij} is introduced once again

$$d_{ij} = \partial_i A_j, \quad (5.67)$$

with the constraint

$$0 = C_{ijk} \equiv \partial_i d_{jk} - \partial_j d_{ik}. \quad (5.68)$$

The evolution system is therefore

$$\partial_t d_{ij} = -\partial_i E_j \quad (5.69)$$

$$\partial_t E_i = -\partial^j d_{ji} + c \partial_i d_{jj} + (1 - c) \partial^j d_{ij} + \partial_i Z \quad (5.70)$$

$$\partial_t Z = \partial^i E_i, \quad (5.71)$$

so that the only difference in P_n is in the scalar block, (d_{nn}, E_n, d_{qq}, Z) :

$$P^n = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 0 & 0 & c & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix},$$

giving a eigenvalue of $\lambda = 0$, which corresponds to the eigenvectors $(1, 0, 0, 0)$ and $(1, 0, 1, -c)$ and eigenvalues $\lambda = \pm 1$ corresponding to $(1, \mp 1, 0, -1)$. The eigenvalues are real and there are a full set of eigenvectors so the system is strongly hyperbolic.

The constraint evolution system can also be constructed in the same way. So far, the constraints are

$$0 = C \equiv \partial^i E_i \tag{5.72}$$

$$0 = Z \tag{5.73}$$

$$0 = C_{ijk} \equiv \partial_i d_{jk} - \partial_j d_{ik}. \tag{5.74}$$

$$\tag{5.75}$$

The time derivative of C is

$$\begin{aligned} \dot{C} &= \partial^i \dot{E}_i \\ &= -\partial^i \partial^j d_{ji} + \partial^i \partial_i d_{jj} + \partial^i \partial_i Z \\ &= Z_{,ii}, \end{aligned} \tag{5.76}$$

from (5.74). Another variable is introduced to reduce the constraint system to first order. W_i is defined as

$$W_i = \partial_i Z, \tag{5.77}$$

with constraint

$$0 = C_{ij} \equiv \partial_j W_i - \partial_i W_j, \tag{5.78}$$

giving

$$\dot{C} = \partial^i \dot{W}_i. \tag{5.79}$$

Also

$$\begin{aligned} \dot{C}_{ijk} &= \partial_i \dot{d}_{jk} - \partial_j \dot{d}_{ik} \\ &= -\partial_i \partial_j E_k + \partial_j \partial_i E_k \\ &= 0 \end{aligned} \tag{5.80}$$

and

$$\begin{aligned}\dot{W}_i &= \partial^j \partial_i E_j \\ &= \partial_i C\end{aligned}\tag{5.81}$$

and

$$\begin{aligned}\dot{C}_{ij} &= \partial_j \dot{W}_i - \partial_i \dot{W}_j \\ &= \partial_i \partial_j C - \partial_j \partial_i C \\ &= 0.\end{aligned}\tag{5.82}$$

So, in summary, the constraint system is

$$\dot{C} = \partial^i W_i\tag{5.83}$$

$$\dot{W}_i = \partial_i C\tag{5.84}$$

$$\dot{C}_{ij} = 0\tag{5.85}$$

$$\dot{C}_{ijk} = 0,\tag{5.86}$$

which has real eigenvalues and a full set of eigenvectors and so is strongly hyperbolic.

Without reducing to first order, the same process can be used but the first derivatives of the magnetic potential that would be rewritten as new variables are instead used directly as evolution variables. This means that there will be no constraint C_{ijk} . The blocks are $(A_{n,n}, E_n, Z)$, $(A_{B,n}, E_B)$ and $(A_{i,B})$. For the scalar block

$$P_n = \begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.$$

The eigenvector for $\lambda = 0$ is $(1, 0, 0)$ and those for $\lambda = \pm 1$ are $(-1, \pm 1)$. For transverse vector block:

$$P_n^\dagger = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$$

and the eigenvectors for $\lambda = \pm 1$ are $(-1, \pm 1)$. The transverse traceless tensor block $A_{i,B}$ will be zero. There is a full set of eigenvectors for P_n . Note that the process in second order form deals with a matrix of size one smaller than when performing a first order reduction, however the row ignored will always be a row of zeros, which will always give the extra eigenvector required.

By taking the inverse of the matrix of eigenvectors, the characteristic variables are

$$U_0 = A_{n,n} + Z \quad (5.87)$$

$$U_{\pm} = Z \pm E_n \quad (5.88)$$

$$U_{\pm B} = -A_{B,n} \pm E_B, \quad (5.89)$$

with speeds zero, ∓ 1 and ∓ 1 respectively (note speed = $-\lambda$.) Again, it should be stressed that multiples of the transverse derivatives can be added to the characteristic variables as the partial derivatives commute, meaning that the time derivative of a transverse derivative will always give a transverse derivative. Finally, the third block $A_{i,B}$ has been neglected here as it is automatically zero speed.

Chapter 6

KWB

6.1 Discrete energy

6.1.1 Discrete energy without boundaries

Initially considering no boundaries to the domain, the system can be discretised in the standard second order accurate way to give

$$\dot{A}_i = -E_i \quad (6.1)$$

$$\dot{E}_i = -D_{+j}D_{-j}A_i + D_{0i}\Gamma \quad (6.2)$$

$$\dot{\Gamma} = 0. \quad (6.3)$$

The energy density can be discretised as

$$2\epsilon_D = c_0(E_i^2 + (D_{+j}A_i)^2 - 2D_{0i}A_i\Gamma) + c_1\Gamma^2 + c_2(D_{0i}A_iD_{0j}A_j - D_{0j}A_iD_{0i}A_j). \quad (6.4)$$

There is always a choice of whether to use D_+ or D_0 for the first derivatives in the energy density but considering summation by parts with no boundaries in Appendix C, the choices made here will allow cancellation when a sum of the energy density is made over the grid.

Making the parameter choices $c_0 = 1$, $c_1 = \sigma$ and $c_2 = 0$ the energy density is

$$2\epsilon_D = E_i^2 + (D_{+j}A_i)^2 - 2D_{0i}A_i\Gamma + \sigma\Gamma^2. \quad (6.5)$$

If we now sum over the grid points, the time derivative of the energy is

$$\begin{aligned} \dot{E}_D &= (E_i, \dot{E}_i) + (D_{+j}A_i, D_{+j}\dot{A}_i) - (D_{0i}A_i, \dot{\Gamma}) - (D_{0i}\dot{A}_i, \Gamma) + (\Gamma, \dot{\Gamma}) \\ &= -(E_i, D_{+j}D_{-j}A_i) + (E_i, D_{0i}\Gamma) - (D_{+i}A_j, D_{+i}E_j) + (D_{0i}E_i, \Gamma). \end{aligned} \quad (6.6)$$

Now making use of summation by parts with no boundaries from Appendix C, this becomes

$$\dot{E}_D = (D_{+j}E_i, D_{+j}A_i) - (D_{0i}E_i, \Gamma) - (D_{+i}A_j, D_{+i}E_j) + (D_{0i}E_i, \Gamma) = 0. \quad (6.7)$$

Hence this energy is conserved.

6.1.2 Positive definite discrete energy without boundaries

Now we show that this energy is positive definite

$$2E_D = (E_i, E_i) + (D_{+j}A_i, D_{+j}A_i) - 2(D_{0i}A_i, \Gamma) + \sigma\|\Gamma\|^2. \quad (6.8)$$

We introduce X ,

$$X = -2(D_{0i}A_i, \Gamma). \quad (6.9)$$

Using the Cauchy-Schwarz inequality, we get

$$X \geq -2\|D_{0i}A_i\|\|\Gamma\| \quad (6.10)$$

and (D.17) gives

$$X \geq -\epsilon\|D_{0i}A_i\|^2 - \epsilon^{-1}\|\Gamma\|^2. \quad (6.11)$$

Now, using $D_0f = \frac{1}{2}(D_+f + D_-f)$,

$$\begin{aligned} \|D_0f\|^2 &= \left\| \frac{1}{2}D_+f + \frac{1}{2}D_-f \right\|^2 \\ &\leq \frac{1}{2}\|D_+f\|^2 + \frac{1}{2}\|D_-f\|^2 \\ &= \|D_+f\|^2, \end{aligned} \quad (6.12)$$

using the triangle inequality and the fact that $\|D_+u\|$ is equivalent to $\|D_-u\|$ with no boundaries. Therefore

$$X \geq -\epsilon\|D_{+i}A_i\|^2 - \epsilon^{-1}\|\Gamma\|^2. \quad (6.13)$$

The derivative $D_{+i}A_j$ is split into trace and tracefree parts

$$S_{ij} \equiv \|D_{+i}A_j\| = \frac{1}{3}\delta_{ij}S_{kk} + \tilde{S}_{ij}. \quad (6.14)$$

Therefore

$$S_{ij}S^{ij} = \frac{1}{3}(S_{kk})^2 + \tilde{S}_{ij}\tilde{S}^{ij} \quad (6.15)$$

and

$$\|D_{+i}A_i\| = S_{kk}, \quad (6.16)$$

so that the full energy

$$\begin{aligned}
E_D &= (E_i, E_i) + (D_{+i}A_j, D_{+i}A_j) - 2(D_{0i}A_i, \Gamma) + \sigma\|\Gamma\|^2 \geq \\
&(E_i, E_i) + \frac{1}{3}(S_{kk})^2 + \tilde{S}_{ij}\tilde{S}^{ij} - \epsilon(S_{kk})^2 - \epsilon^{-1}\|\Gamma\|^2 + \sigma\|\Gamma\|^2 = \\
&(E_i, E_i) + \left(\frac{1}{3} - \epsilon\right)(S_{kk})^2 + \tilde{S}_{ij}\tilde{S}^{ij} + (\sigma - \epsilon^{-1})\|\Gamma\|^2, \tag{6.17}
\end{aligned}$$

which is positive definite for $\epsilon \leq \frac{1}{3}$ and therefore $\sigma \geq 3$. So, in summary, if we define the vector $u = (E_i, D_{+i}A_j, \Gamma)$ then we have a conserved energy E constructed of quadratic forms of $(E_i, D_{+i}A_j, D_{0i}A_j, \Gamma)$ with

$$\dot{E} = 0, \tag{6.18}$$

such that

$$E \geq K^2\|u\|^2 \tag{6.19}$$

and therefore

$$E^{\frac{1}{2}} \geq K\|E_i\| \quad E^{\frac{1}{2}} \geq K\|D_{+i}A_j\| \quad E^{\frac{1}{2}} \geq K\|\Gamma\|. \tag{6.20}$$

The solution $\|u(t)\|$ is bounded by $E^{\frac{1}{2}}/K$, which is constant and so it can always be bounded by the initial data, giving the stability estimate required

$$\|u(t)\| \leq K_1\|u(0)\|. \tag{6.21}$$

6.1.3 Lower order terms

Now consider the lower order term A_i that is missing from energy E . This must be included to give a positive definite energy in all the evolution variables. By simply adding an A_i^2 term to the energy with an arbitrary coefficient, the energy will no longer be conserved but will be positive definite in all evolution variables. That is

$$\epsilon_{\text{full}} = E_i^2 + (D_{+i}A_j)^2 - 2D_{0i}A_i\Gamma + \sigma\Gamma^2 + \alpha^2A_i^2. \tag{6.22}$$

Let $u = (E_i, A_i, D_{+i}A_j, \Gamma)$. Therefore we have

$$E_{\text{full}} \geq K_2\|u\|^2 \tag{6.23}$$

but E_{full} is not now conserved. However,

$$\begin{aligned}
\dot{E}_{\text{full}} &\leq -2\alpha^2(A_i, E_i) \\
&\leq \alpha^2(\|A_i\|^2 + \|E_i\|^2) \\
&\leq \alpha^2\|u\|^2 \\
&\leq \alpha^2K_2^{-1}E. \tag{6.24}
\end{aligned}$$

So, the increase in energy is bounded by the energy itself and hence

$$E(t) \leq e^{\alpha^2 t/K_2} E(0), \quad (6.25)$$

which is the stability estimate required.

$$\begin{aligned} \|u(t)\| \leq E_{\text{full}} &\leq e^{\alpha^2 t/K_2} E(0) \\ &\leq K e^{\alpha^2 t/K_2} \|u(0)\|, \end{aligned} \quad (6.26)$$

where $K\|u(0)\| = E(0)$. The efficiency of the estimate can be improved by reducing the value of α .

6.1.4 Discrete energy with a boundary

Introducing a boundary requires using the MDBC; we consider the boundary at $j = N$. The characteristic variables are

$$U_{\pm} = -\partial_n A_n \pm E_n + \Gamma \quad (6.27)$$

$$U_{\pm B} = -\partial_n A_B \pm E_B, \quad (6.28)$$

so recalling the technique used for the second order wave equation in Section 3.2.1, we substitute the characteristic variables into the MDBC and make a second order difference approximation for the first derivative

$$D_{0n} A_n = \partial_n A_n \doteq \frac{1 + \kappa_s}{1 - \kappa_s} E_n + \Gamma - \frac{f_n}{1 - \kappa_s} \quad (6.29)$$

$$D_{0n} A_B = \partial_n A_B \doteq \frac{1 + \kappa_v}{1 - \kappa_v} E_B - \frac{f_B}{1 - \kappa_v} \quad (6.30)$$

and hence write $D_+ D_-$ as

$$D_+ D_- = \frac{2}{h} (D_0 - D_-) = \frac{2}{h} (D_+ - D_0) \quad (6.31)$$

to obtain the semi-discrete ODE's on the boundary

$$\dot{A}_i \doteq -E_i \quad (6.32)$$

$$\begin{aligned} \dot{E}_n &\doteq \frac{2}{h} D_{-n} A_n + \frac{2}{h} \left[-\frac{1 + \kappa_s}{1 - \kappa_s} E_n - \Gamma + \frac{f_n}{1 - \kappa_s} \right] \\ &\quad - D_{+B} D_{-B} A_n + D_{-n} \Gamma \end{aligned} \quad (6.33)$$

$$\begin{aligned} \dot{E}_B &\doteq \frac{2}{h} D_{-n} A_B + \frac{2}{h} \left[-\frac{1 + \kappa_v}{1 - \kappa_v} E_B + \frac{f_B}{1 - \kappa_v} \right] \\ &\quad - D_{+C} D_{-C} A_B + D_{0B} \Gamma \end{aligned} \quad (6.34)$$

$$\dot{\Gamma} \doteq 0, \quad (6.35)$$

where we have taken a one-sided derivative for Γ in the evolution equation for E_n . This is synonymous with second order extrapolation, i.e. setting the second spatial derivative at the boundary to zero

$$\Gamma_{-1} - 2\Gamma_0 + \Gamma_1 = 0. \quad (6.36)$$

The boundary at $j = 0$ is calculated in a similar way

$$\begin{aligned} \dot{E}_n &\doteq -\frac{2}{h}D_{+n}A_n - \frac{2}{h}\left[\frac{1+\kappa_s}{1-\kappa_s}E_n - \Gamma + \frac{f_n}{1-\kappa_s}\right] \\ &\quad - D_{+B}D_{-B}A_n + D_{-n}\Gamma \end{aligned} \quad (6.37)$$

$$\begin{aligned} \dot{E}_B &\doteq -\frac{2}{h}D_{+n}A_B - \frac{2}{h}\left[\frac{1+\kappa_v}{1-\kappa_v}E_B + \frac{f_B}{1-\kappa_v}\right] \\ &\quad - D_{+C}D_{-C}A_B + D_{0B}\Gamma \end{aligned} \quad (6.38)$$

We now consider the energy including the boundary terms. For simplicity we restrict ourselves to the half plane problem with a boundary at $j = 0$ so that $x \geq 0$. The calculation works in the same way for a boundary at $j = N$.

The summation by parts rules will be used again but with boundary terms included (see Appendix C). The bulk energy will be the same as above but the scalar product will now be the sum over $j = 1, 2, \dots$. Boundary terms at $j = 0$ can then be added in a consistent way. Hence the bulk energy density is

$$2E_{\text{bulk}} = (E_i, E_i) + (D_{+j}A_i, D_{+j}A_i) - 2(D_{0i}A_i, \Gamma) + \sigma\|\Gamma\|^2. \quad (6.39)$$

We use summation by parts on the derivatives in the periodic directions (i.e. D_B) in the same way as above so these terms will still vanish.

$$\begin{aligned} \dot{E}_{\text{bulk}} &= -(E_i, D_{+j}D_{-j}A_i)_1^\infty + (E_i D_{0i}, \Gamma) - (D_{+i}A_j D_{+i}, E_j) + (D_{0i}E_i, \Gamma) \\ &= -(D_{+j}E_i, D_{+j}A_i) + (E_i D_{0i}, \Gamma) - (D_{+i}A_j D_{+i}, E_j) + (D_{0i}E_i, \Gamma) \\ &= hE_i^1 D_{+n}A_i^0 - \frac{1}{2}E_n^1 \Gamma^0 - \frac{1}{2}E_n^0 \Gamma^1, \end{aligned} \quad (6.40)$$

noting that the superscripts indicate the grid position.

The boundary terms that we will add onto the bulk energy will be those that have the correct summation property when adding two touching boundaries together from separate domains. The first term we add is $\frac{h}{2}E_i^2$ as there will be a contribution from each of the domain boundaries giving a total of hE_i^2 . The second term we add is $\frac{h}{2}(D_{+B}A_j)^2 + h(D_{+n}A_j)^2$ because the transverse derivative will have a contribution from both boundaries whilst the normal derivative will only have one contribution from the domain in which it lies. The last term we add is

$-hD_B A_B \Gamma - hD_{+n} A_n \Gamma$. There will be a contribution to the transverse derivative from both boundaries giving the correct coefficient of $-2h$ but there will also be a contribution to the normal derivative from the other boundary, where the boundary term will be $-hD_{-n} A_n \Gamma$, which when added to $-hD_{+n} A_n \Gamma$ gives $-2hD_{0n} A_n \Gamma$ as $D_+ + D_- = 2D_0$.

$$2E_{\text{bnd}} \doteq \frac{h}{2} E_i^2 + \frac{h}{2} (D_{+B} A_j)^2 + h (D_{+n} A_j)^2 - h D_{0B} A_B \Gamma - h D_{+n} A_n \Gamma \quad (6.41)$$

and therefore substituting in the boundary equations (6.37) and (6.38)

$$\begin{aligned} \dot{E}_{\text{bnd}} &\doteq \frac{h}{2} E_n \left[-\frac{2}{h} D_{+n} A_n + \frac{2}{h} \left(-\frac{1 + \kappa_s}{1 - \kappa_s} E_n + \Gamma - \frac{f_n}{\kappa_s} \right) - D_{+B} D_{-B} A_n + D_{+n} \Gamma \right] \\ &\quad + \frac{h}{2} E_B \left[-\frac{2}{h} D_{+n} A_B + \frac{2}{h} \left(-\frac{1 + \kappa_v}{1 - \kappa_v} E_B - \frac{f_B}{1 - \kappa_v} \right) - D_{+B} D_{-B} A_B + D_{+B} \Gamma \right] \\ &\quad - \frac{h}{2} D_{+B} A_j D_{+B} E_j - h D_{+n} A_j D_{+n} E_j + \frac{h}{2} D_{0B} E_B \Gamma_0 + \frac{h}{2} D_{+n} E_n^0 \Gamma_0 \\ &= -E_n \frac{E^n (1 + \kappa_s) - f_n}{1 - \kappa_s} - E_B \frac{E^B (1 + \kappa_v) - f_B}{1 - \kappa_v} - E_i D_{+n} A_i + E_n \Gamma \\ &\quad - \frac{h}{2} E_i D_{+B} D_{-B} A_i + \frac{h}{2} E_n D_{+n} \Gamma + \frac{h}{2} E_B D_{0B} \Gamma - \frac{h}{2} D_{+B} A_j D_{+B} E_j \\ &\quad - h D_{+n} A_j D_{+n} E_j + \frac{h}{2} D_{0B} E_B \Gamma + \frac{h}{2} D_{+n} E_n \Gamma. \end{aligned} \quad (6.42)$$

Hence adding together equations (6.40) and (6.42) gives

$$\begin{aligned} \dot{E}_{\text{bulk}} + \dot{E}_{\text{bnd}} &= - \left[\frac{1 + \kappa}{1 - \kappa} (E_i^0)^2 - \frac{E_i^0 f_n}{1 - \kappa} \right] \\ &= - \left(\frac{1}{1 - \kappa_s^2} \right) \left[(1 + \kappa_s) E_n^0 + \frac{f_n}{2} \right]^2 + \frac{1}{4} \left(\frac{f_n^2}{1 - \kappa_s^2} \right), \end{aligned} \quad (6.43)$$

which is non-increasing for $f_i = 0$ as expected.

6.1.5 Positive definite discrete energy with a boundary

We now show that this energy is still positive definite. We recall that the energy is

$$\begin{aligned} 2E_D &= (E_i, E_i) + (D_{+j} A_i, D_{+j} A_i) - 2(D_{0i} A_i, \Gamma) + \sigma \|\Gamma\|^2 \\ &\quad + \frac{h}{2} E_i^0 E_i^0 + \frac{h}{2} D_{+B} A_j^0 D_{+B} A_j^0 + h D_{+n} A_j^0 D_{+n} A_j^0 - h D_{0B} A_B^0 \Gamma^0 \\ &\quad - h D_{+n} A_n^0 \Gamma^0 + \frac{h}{2} \sigma (\Gamma^0)^2. \end{aligned} \quad (6.44)$$

For simplicity, the energy is split into a component only involving normal derivatives of A_i

$$2E_N = (D_{+n}A_i, S_{+n}A_i) - 2(D_{0n}A_n, \Gamma) + \sigma_1 \|\Gamma\|^2 + \hbar D_{+n}A_i^0 D_{+n}A_i^0 - \hbar D_{+n}A_n^0 \Gamma^0 + \frac{\hbar}{2} \sigma_1 (\Gamma^0)^2 \quad (6.45)$$

and a component involving the transverse derivatives of A_i and the E_i terms

$$2E_T = (E_i, E_i) + (D_{+B}A_j, D_{+B}A_j) - 2(D_{0B}A_B, \Gamma) + \sigma_2 \|\Gamma\|^2 + \frac{\hbar}{2} E_i^0 E_i^0 + \frac{\hbar}{2} D_{+B}A_j^0 D_{+B}A_j^0 - \hbar D_{0B}A_B^0 \Gamma^0 + \frac{\hbar}{2} \sigma_2 (\Gamma^0)^2. \quad (6.46)$$

From equation (6.13)

$$-2(D_{0B}A_B, \Gamma) \geq -\epsilon_T \|D_{+B}A_B\|^2 - \epsilon_T^{-1} \|\Gamma\|^2 \quad (6.47)$$

because there are still no boundaries in the transverse direction. Once again the derivative $D_{+B}A_C$ is split into trace and tracefree parts

$$S_{BC} \equiv \|D_{+B}A_C\| = \frac{1}{2} \delta_{BC} S_{DD} + \tilde{S}_{BC}, \quad (6.48)$$

to give

$$(D_{+B}A_C, D_{+B}A_C) = S_{BC} S^{BC} = \frac{1}{2} S_{DD}^2 + \tilde{S}_{BC} \tilde{S}^{BC} \quad (6.49)$$

and

$$\|D_{+B}A_B\|^2 = S_{BB}^2, \quad (6.50)$$

so that

$$\begin{aligned} (D_{+B}A_C, D_{+B}A_C) - 2(D_{0B}A_B, \Gamma) &\geq \tilde{S}_{BC} \tilde{S}_{BC} + \left(\frac{1}{2} - \epsilon_T\right) S_{BB} S^{BB} - \epsilon_T^{-1} \|\Gamma\|^2 \\ &\geq \left(\frac{1}{2} - \epsilon_T\right) (D_{+B}A_C, D_{+B}A_C) - \epsilon_T^{-1} \|\Gamma\|^2. \end{aligned} \quad (6.51)$$

Also considering the boundary terms, the same technique can be used for the associated terms giving

$$\frac{\hbar}{2} D_{+B}A_C^0 D_{+B}A_C^0 - \hbar D_{0B}A_B^0 \Gamma^0 \geq \left(\frac{1}{2} - \epsilon_T\right) \frac{\hbar}{2} D_{+B}A_C^0 D_{+B}A_C^0 - \epsilon_T^{-1} \hbar (\Gamma^0)^2. \quad (6.52)$$

Therefore

$$\begin{aligned} 2E_T &\geq (E_i, E_i) + (D_{+B}A_n, D_{+B}A_n) \\ &\quad + \left(\frac{1}{2} - \epsilon_T\right) (D_{+B}A_C, D_{+B}A_C) + (\sigma_2 - \epsilon_T^{-1}) \|\Gamma\|^2 \\ &\quad + \frac{\hbar}{2} \left[E_i^0 E_i^0 + D_{+B}A_n^0 D_{+B}A_n^0 + \left(\frac{1}{2} - \epsilon_T\right) D_{+B}A_C^0 D_{+B}A_C^0 + (\sigma_2 - \epsilon_T^{-1}) (\Gamma^0)^2 \right] \end{aligned} \quad (6.53)$$

and E_T is positive definite for $\epsilon_T \leq \frac{1}{2}$ and therefore $\sigma_2 \geq 2$.

$$\begin{aligned} 2E_N &= (D_{+n}A_i, D_{+n}A_i) - 2(D_{0n}A_n, \Gamma) + \sigma_1 \|\Gamma\|^2 \\ &\quad + hD_{+n}A_{i0}D_{+n}A_i^0 - hD_{+n}A_n^0\Gamma^0 + \frac{h}{2}\sigma_1(\Gamma^0)^2. \end{aligned} \quad (6.54)$$

Once again, the same process can be used, however this time the relation

$$\|D_0f\| \leq \|D_+f\|, \quad (6.55)$$

is invalid as there is no summation to infinity. However the relation

$$\|D_0f\|_1^\infty \leq \|D_+f\|_0^\infty, \quad (6.56)$$

is true as

$$\|D_-f\|_1^\infty = \|D_+f\|_0^\infty. \quad (6.57)$$

Therefore, by adding one of the boundary terms to a bulk term the same argument holds

$$\begin{aligned} &\frac{1}{2}(\|D_{+n}A_n\|^2 + h(D_{+n}A_n^0)^2) - 2(D_{0n}A_n, \Gamma) + \sigma_1 \|\Gamma\|^2 \\ &\geq \left(\frac{1}{2} - \epsilon_N\right)(\|D_{+n}A_n\|^2 + h(D_{+n}A_n^0)^2) + \left(\sigma_1 - \frac{1}{\epsilon_N}\right)\|\Gamma\|^2 \end{aligned} \quad (6.58)$$

and

$$\begin{aligned} &\frac{h}{2}((D_{+n}A_n^0)^2 - 2(D_{+n}A_n^0\Gamma^0) + \sigma_1(\Gamma^0)^2) \\ &\geq \frac{h}{2}(1 - \epsilon_B)(D_{+n}A_n^0)^2 + \left(\sigma_1 - \frac{1}{\epsilon_B}\right)(\Gamma^0)^2 \end{aligned} \quad (6.59)$$

and therefore the normal part gives

$$\begin{aligned} 2E_N &\geq \left(\frac{1}{2} - \epsilon_N\right)(\|D_{+n}A_n\|^2 + h(D_{+n}A_n^0)^2) + \left(\sigma_1 - \frac{1}{\epsilon_N}\right)\|\Gamma\|^2 \\ &\quad + \frac{h}{2}(1 - \epsilon_B)(D_{+n}A_n^0)^2 + \left(\sigma_1 - \frac{1}{\epsilon_B}\right)(\Gamma^0)^2 \\ &\quad + \frac{1}{2}\|D_{+n}A_n\|^2 + (D_{+n}A_B, D_{+n}A_B) + hD_{+n}A_B^0D_{+n}A_B^0, \end{aligned} \quad (6.60)$$

which is positive definite for

$$\frac{1}{2} > \epsilon_N \Rightarrow \sigma_1 > 2 \quad (6.61)$$

and

$$1 > \epsilon_B \Rightarrow \sigma_1 > 1. \quad (6.62)$$

Finally putting all these sections together provides the inequality on the whole energy

$$\begin{aligned}
2E \geq & (E_i, E_i) + (D_{+i}A_j, D_{+i}A_j) - \frac{1}{2}(D_{+B}A_C, D_{+B}A_C) - \epsilon_T(D_{+B}A_C, D_{+B}A_C) \\
& - \epsilon_N \|D_{+n}A_n\|^2 + (\sigma_1 + \sigma_2 - \frac{1}{\epsilon_N} - \frac{1}{\epsilon_T}) \|\Gamma\|^2 \\
& + \frac{\hbar}{2} [E_i^0 E_i^0 + D_{+i}A_j^0 D_{+i}A_j^0 + D_{+n}A_i^0 D_{+n}A_i^0 \\
& - (\frac{1}{2} + \epsilon_T) D_{+B}A_C^0 D_{+B}A_C^0 - (2\epsilon_N + \epsilon_B)(D_{+n}A_n^0)^2 \\
& + (\sigma_2 + \sigma_1 - \epsilon_T^{-1} - \epsilon_B^{-1})(\Gamma^0)^2], \tag{6.63}
\end{aligned}$$

which is positive definite for the conditions given above.

6.2 Constraint preserving boundary conditions for the KWB system

Constraint preserving boundary conditions can be applied as described above. The constraint system for KWB can be written in closed form as

$$\dot{C} = (C_{\Gamma,n})_{,n} + (C_{\Gamma,B})_{,B} \tag{6.64}$$

$$\dot{C}_{\Gamma,n} = C_{,n}, \tag{6.65}$$

which (neglecting transverse derivatives) is just the first order in space wave equation and hence the characteristic variables are

$$C_+ = C_{\Gamma,n} + C = \partial_n(\Gamma - \partial^i A_i) + \partial^i E_i \tag{6.66}$$

$$C_- = C_{\Gamma,n} - C = \partial_n(\Gamma - \partial^i A_i) - \partial^i E_i \tag{6.67}$$

and therefore, writing in terms of characteristic variables

$$C_+ = \partial_i U_{+i} \tag{6.68}$$

$$C_- = \partial_i U_{-i} \tag{6.69}$$

and the constraint energy can be controlled by applying ‘homogeneous maximally dissipative boundary conditions’ to C_{\pm}

$$C_+ - \kappa_c C_- = 0. \tag{6.70}$$

Substituting (6.68) and (6.69) into (6.70) gives

$$\partial_n U_+ + \partial^A U_{+A} - \kappa_c (\partial_n U_- + \partial^A U_{-A}) = 0. \tag{6.71}$$

The evolution equations for the characteristic variables

$$\partial_t U_+ = E_{n,n} - A_{n,jj} + \Gamma_{,n} = (U_+)_{,n} - A_{n,BB} \quad (6.72)$$

$$\partial_t U_- = E_{n,n} + A_{n,jj} - \Gamma_{,n} = -(U_-)_{,n} + A_{n,BB} \quad (6.73)$$

can be used to give the form

$$\partial_t(U_+ + \kappa_c U_-) = -\partial^A U_{+A} + \kappa_c \partial^A U_{-A} - (1 - \kappa_c) \partial^A \partial_A A_n. \quad (6.74)$$

A new variable $X = U_+ + \kappa_c U_-$, which is defined only on the boundary, can be used as the free data in the first of the three maximally dissipative boundary conditions

$$U_+ - \kappa_s U_- = f, \quad (6.75)$$

with $\kappa_s = -\kappa_c$ and $f = X$. We use κ_s and κ_v as the coupling constants corresponding to the first MDBC and the remaining two MDBC respectively. These two remaining MDBC are used to give the evolution equation for X in terms of transverse derivatives of the evolution variables (equation 6.76). X can be specified in the initial data as $X = U_+ - \kappa_s U_-$ and evolved using

$$\begin{aligned} \dot{X} &= -\partial^B(-A_{B,n} + E_B) + \kappa_c \partial^B(-A_{B,n} - E_B) - (1 - \kappa_c) \partial^B \partial_B A_n \\ &= \frac{1 - \kappa_c}{\kappa_v - 1} \left(\partial^B f_B - (1 + \kappa_v) \partial^B E_B \right) - (1 + \kappa_c) \partial^B E_B - (1 - \kappa_c) \partial^B \partial_B A_n \\ &= \frac{1 + \kappa_s}{\kappa_v - 1} \partial^B f_B - 2 \frac{\kappa_s + \kappa_v}{\kappa_v - 1} \partial^B E_B - (1 + \kappa_s) \partial^B \partial_B A_n. \end{aligned} \quad (6.76)$$

The standard second order accurate discretisation of \dot{X} is

$$\dot{X} = \frac{1 + \kappa_s}{\kappa_v - 1} D_{0B} f_B - 2 \frac{\kappa_s + \kappa_v}{\kappa_v - 1} D_{0B} E_B - (1 + \kappa_s) D_{+B} D_{-B} A_n. \quad (6.77)$$

6.3 The KWB system with shift

Taking the KWB evolution equations (5.35 - 5.37), we now make a Galilean transformation to incorporate a shift into these evolution equations. We set

$$t = \tilde{t} \quad (6.78)$$

$$x^i = \tilde{x}^i - \beta^i \tilde{t} \quad (6.79)$$

and hence

$$\frac{\partial}{\partial \tilde{t}} = \frac{\partial}{\partial t} - \beta^i \frac{\partial}{\partial x^i} \quad (6.80)$$

$$\frac{\partial}{\partial \tilde{x}^i} = \frac{\partial}{\partial x^i}. \quad (6.81)$$

Therefore, the evolution equations become

$$\dot{A}_i = \beta^i \partial_i A_i - E_i \quad (6.82)$$

$$\dot{E}_i = \beta^i \partial_i E_i - \partial^j \partial_j A_i + \partial_i \Gamma \quad (6.83)$$

$$\dot{\Gamma} = \beta^i \partial_i \Gamma, \quad (6.84)$$

where the dot now stands for the derivative with respect to \tilde{t} . We can let $\partial_0 = \partial_{\tilde{t}} - \beta^i \partial_i$ to give,

$$\partial_0 A_i = -E_i \quad (6.85)$$

$$\partial_0 E_i = -\partial^j \partial_j A_i + \partial_i \Gamma \quad (6.86)$$

$$\partial_0 \Gamma = 0, \quad (6.87)$$

where the constraints and the characteristic variables remain the same but where the latter have different characteristic speeds. That is

$$0 = C_E \equiv E_{i,i} \quad (6.88)$$

$$0 = C_\Gamma \equiv \Gamma - A_{j,j}, \quad (6.89)$$

$$U_\pm = -A_{n,n} \pm E_n + \Gamma \quad (6.90)$$

$$U_{\pm B} = -A_{B,n} \pm E_B, \quad (6.91)$$

with eigenvalues $\lambda = \beta^n \pm 1$. The evolution equations of the characteristic variables are

$$\dot{U}_\pm = (\beta^n \pm 1)U_{\pm,n} + \beta^A U_{\pm,A} \mp A_{n,BB}. \quad (6.92)$$

We restrict to $|\beta^n| < 1$. With $\beta^n = 0$, we have already seen that Γ is a zero-speed variable. Γ will be incoming for $\beta^n > 0$ and outgoing for $\beta^n < 0$, with $\lambda = \beta$. For completeness, the case where $\beta = 1$ will cause the usual incoming characteristics to become zero speed and the case where $|\beta| > 1$ will ensure that the seven characteristics have the same direction, however, we will not consider these alternative situations.

6.3.1 Exact solution for the KWB system with shift

We now consider an exact solution for this system of equations. As we only have a boundary in the x -direction, the wave vector in that direction k_n will be broken down into components associated with ingoing, outgoing and ‘parallel to the

boundary' waves, k_{+n} , k_{-n} and k_{0n} respectively. Normally, we calculate $\omega = |k_i|^2$ from the specified wave vectors k_i . However, in this case, we want to consider the solutions with respect to the boundary and hence we fix the transverse wave vector, k_A , and ω , and calculate incoming, outgoing and parallel to the boundary wave vectors, k_{\pm} and k_0 respectively. We introduce the shorthand $\psi = \exp[i(k_A Y^A - \omega t)]$ and the solutions $\psi_0 = \psi \exp[i(k_{0n} X)]$ and $\psi_{\pm} = \psi \exp[i(k_{\pm n} X)]$, which are the parallel, ingoing and outgoing solutions, which we desire to satisfy the shifted transport and wave equations respectively. Now

$$\partial_0 \psi_{\pm} = -i(\omega + \beta^n k_{\pm n} + \beta^A k_A) \psi_{\pm} \quad (6.93)$$

and hence we introduce the notation $\omega_{\pm} = \omega + \beta^n k_{\pm n} + \beta^A k_A$ so that

$$\partial_0 \psi_{\pm} = -i\omega_{\pm} \psi_{\pm} \quad \text{and} \quad \partial_0^2 \psi_{\pm} = -\omega_{\pm}^2 \psi_{\pm} \quad (6.94)$$

and

$$\partial^j \partial_j \psi_{\pm} = -(k_A k^A + k_{\pm n}^2) \psi_{\pm}. \quad (6.95)$$

So, to ensure that ψ_{\pm} satisfies the shifted wave equation

$$\partial_0^2 \psi_{\pm} = \partial_j \partial^j \psi_{\pm}, \quad (6.96)$$

we need

$$(\omega + \beta^n k_{\pm n} + \beta^A k_A)^2 = k_A k^A + k_{\pm n}^2. \quad (6.97)$$

Rewriting this expression to give $k_{\pm n}$ in terms of ω and β^i , we have

$$k_{\pm n} = \frac{\beta^n (\omega + \beta^A k_A)}{1 - \beta^{n2}} \mp \frac{[(\omega + \beta^A k_A)^2 - k_A k^A (1 - \beta^{n2})]^{\frac{1}{2}}}{1 - \beta^{n2}}. \quad (6.98)$$

Note that because $k_{\pm n}$ are complex, we ensure that the values of k_A and ω that we choose will give a real result. The parallel wave vector

$$\partial_0 \psi_0 = 0, \quad (6.99)$$

implies that

$$\omega + \beta^n k_{0n} + \beta^A k_A = 0 \quad (6.100)$$

or

$$k_{0n} = -\frac{1}{\beta^n} (\omega + \beta^A k_A). \quad (6.101)$$

As $\beta^n \rightarrow 0$, k_{0n} would become undesirably large. If $\beta^n = 0$, k_{0n} decouples from ω and k_A , allowing any value to be taken.

Considering the fact that $\partial_0 \Gamma = 0$, we set $\Gamma = m\psi_0$ and

$$A_i = g_{+i}\psi_+ + g_{-i}\psi_- + h_i\psi_0, \quad (6.102)$$

where $g_{\pm i}$, h_i are complex coefficients. Now

$$-\partial_0 A_i = E_i = +g_{+i}i\omega_+\psi_+ + g_{-i}i\omega_-\psi_- - \partial_0 h_i \quad (6.103)$$

and hence, using $\partial_0 E_i = -\partial^j \partial_j A_i + \partial_i \Gamma$,

$$h_i = -\frac{imk_{0i}}{k_{0i}k^{0i}}, \quad (6.104)$$

where $k_{0i} = (k_{0n}, k_A)$ and similarly $k_{\pm i} = (k_{\pm n}, k_A)$, giving the full exact solution in complex form

$$A_i = g_{+i}\psi_+ + g_{-i}\psi_- - ik_{0i}^{-2}k_{0i}m\psi_0 \quad (6.105)$$

$$E_i = i\omega_+g_{+i}\psi_+ + i\omega_-g_{-i}\psi_- \quad (6.106)$$

$$\Gamma = m\psi_0. \quad (6.107)$$

Now we let $\text{Re}(g) = a$, $i\text{Im}(g) = b$, $\text{Re}(m) = c$, $i\text{Im}(m) = d$ and take the real part of the solution, using the notation $\cos \alpha_{\pm,0} = \cos(k_{\pm,0}X + k_A Y^A + \omega t)$ and $\sin \alpha_{\pm,0} = \sin(k_{\pm,0}X + k_A Y^A + \omega t)$

$$\begin{aligned} A_i &= a_{+i} \cos \alpha_+ + b_{+i} \sin \alpha_+ + a_{-i} \cos \alpha_- + b_{-i} \sin \alpha_- \\ &\quad - k_{0i}^{-2}k_{0i}d \cos \alpha_0 + k_{0i}^{-2}k_{0i}c \sin \alpha_0 \end{aligned} \quad (6.108)$$

$$E_i = -\omega_+b_{+i} \cos \alpha_+ + \omega_+a_{+i} \sin \alpha_+ - \omega_-b_{-i} \cos \alpha_- + \omega_-a_{-i} \sin \alpha_- \quad (6.109)$$

$$\Gamma = c \cos \alpha_0 + d \sin \alpha_0. \quad (6.110)$$

If we now consider the constraint preserving boundary condition $C_+ = 0$, we can see that the parameters c and d are not specified by this boundary condition.

$$\begin{aligned} C_+ &\equiv \partial^i E_i + \partial_n(\Gamma - \partial^i A_i) \\ &= \omega_+g_{+i}k_{+i}\psi_+ + \omega_-g_{-i}k_{-i}\psi_- + imk_{0n}\psi_0 \\ &= k_{+n}k_{+i}g_{+i}\psi_+ + k_{-n}k_{-i}g_{-i}\psi_- - imk_{0n}\psi_0 \\ &= g_{+i}k_{+i}(\omega_+ + k_{+n})\psi_+ + g_{-i}k_{-i}(\omega_- + k_{-n})\psi_- = 0. \end{aligned} \quad (6.111)$$

The coefficients of c and d cancel, meaning that the variable Γ is independent of this CPBC. Also note that the full CPBC

$$C_+ = \kappa C_-, \quad (6.112)$$

results in

$$\frac{1-\kappa}{1+\kappa}\partial^i E_i + \partial_n \Gamma - \partial_n \partial^i A_i = 0 \quad (6.113)$$

and as c and d only appear in the 2nd and 3rd terms they will still cancel. At the boundary $x = 0$, $\psi_+ = \psi_- = \psi_0$ and the CPBC holds for arbitrary Y^A and t , so the ψ 's can be cancelled to give

$$g_{+i}k_{+i}(\omega_+ + k_{+n}) + g_{-i}k_{-i}(\omega_- + k_{-n}) = 0. \quad (6.114)$$

It is straightforward to translate this equation into conditions for the real and imaginary parts of the coefficients $g_{\pm i}$

$$(a_{+n}k_{+n} + a_{+B}k_B)(\omega_+ + k_{+n}) + (a_{-n}k_{-n} + a_{-B}k_B)(\omega_- + k_{-n}) = 0 \quad (6.115)$$

$$(b_{+n}k_{+n} + b_{+B}k_B)(\omega_+ + k_{+n}) + (b_{-n}k_{-n} + b_{-B}k_B)(\omega_- + k_{-n}) = 0. \quad (6.116)$$

The simplest way to satisfy the constraints is therefore to set $a_{+i}k_i = 0$, $a_{-i}k_i = 0$, $b_{+i}k_i = 0$ and $b_{-i}k_i = 0$.

The cancellation of c and d also occurs for the non-standard boundary condition

$$\begin{aligned} C_\Gamma &\equiv \Gamma - \partial^i A_i \\ &= m\psi_0 - ik_{+i}g_{+i}\psi_+ - ik_{-i}g_{-i}\psi_- - m\psi_0 = 0 \end{aligned} \quad (6.117)$$

and again at the boundary, this reduces to

$$k_{+i}g_{+i} + k_{-i}g_{-i} = 0 \quad (6.118)$$

and hence

$$a_{+n}k_{+n} + a_{+B}k_B + a_{-n}k_{-n} + a_{-B}k_B = 0 \quad (6.119)$$

$$b_{+n}k_{+n} + b_{+B}k_B + b_{-n}k_{-n} + b_{-B}k_B = 0. \quad (6.120)$$

These conditions provide a simple way of showing that we cannot impose both $C_\Gamma = 0$ and $C_+ = 0$. Consider substituting (6.118) into (6.114) to obtain

$$g_{-i}k_{-i}(\omega_- - \omega_+ + k_{-n} - k_{+n}) = 0, \quad (6.121)$$

which means that given two outgoing modes the remaining one can be calculated. This gives an over-specification of the solution, as from two coefficients, all six coefficients can be calculated, where there should be three degrees of freedom for the three incoming modes.

6.3.2 MDBC for the KWB system with shift

The natural discretisation of the evolution equations for the bulk is

$$\dot{A}_i = \beta^j D_{0j} A_i - E_i \quad (6.122)$$

$$\dot{E}_i = \beta^j D_{0j} E_i - D_{+j} D_{-j} A_i + D_{0i} \Gamma \quad (6.123)$$

$$\dot{\Gamma} = \beta^j D_{0j} \Gamma. \quad (6.124)$$

The first step in discretising the boundaries is to apply maximally dissipative boundary conditions to all the incoming modes. Assuming β^n is positive, these will be U_+ , U_{+B} and Γ (if β^n was negative Γ would be an outgoing variable). MDBC work in exactly the same way as with zero shift; $A_{n,n}$ and $A_{B,n}$ can be calculated analytically from the MDBC

$$U_+ \doteq \kappa_s U_- + f_n \quad (6.125)$$

$$U_{+B} \doteq \kappa_v U_{-B} + f_B, \quad (6.126)$$

giving

$$A_{n,n} \doteq \frac{1 + \kappa_s}{\kappa_s - 1} E_n + \frac{f_n}{\kappa_s - 1} + \Gamma \quad (6.127)$$

$$A_{B,n} \doteq \frac{1 + \kappa_v}{\kappa_v - 1} E_B + \frac{f_B}{\kappa_v - 1}, \quad (6.128)$$

which can be used as a second order approximation for $D_{0n} A_i$. These will give three boundary conditions, whereas there are four incoming modes. Hence we need one more boundary condition and as the remaining incoming mode is Γ , it makes sense to provide a boundary condition on this variable, which can be of the same maximally dissipative form (there is no coupling constant because there is no corresponding outgoing characteristic variable).

$$\Gamma \doteq g. \quad (6.129)$$

where g is the free incoming data. We calculate the first derivatives of E_i by extrapolation. The simplest method for coding purposes is to use the time derivative of g , setting $\dot{\Gamma} \doteq \dot{g}$. This leaves a spatial derivative of Γ to be calculated as part of the right-hand side for E_n , however this can either be found through extrapolation or an algebraic manipulation of $\dot{\Gamma} = \dot{g} = \beta^i \partial_i \Gamma$. This then gives all the derivatives required for the evolution equations. The discretisation of the evolution equations at the boundaries is

$$\dot{A}_n \doteq \beta^n \left(\frac{-(1 + \kappa_s)}{\kappa_s - 1} E_n + \frac{f_n}{\kappa_s - 1} + \Gamma \right) + \beta^C D_{0C} A_n - E_n \quad (6.130)$$

$$\dot{A}_B \doteq \beta^n \left(\frac{-(1 + \kappa_v)}{\kappa_v - 1} E_B + \frac{f_B}{\kappa_v - 1} \right) + \beta^C D_{0C} A_B - E_B \quad (6.131)$$

$$\begin{aligned} \dot{E}_n &= \beta^n D_{-n} E_n - \frac{2}{h} \left[-D_{-n} A_n - \frac{\kappa_s + 1}{\kappa_s - 1} E_n + \frac{f_n}{\kappa_s - 1} + \Gamma \right] \\ &\quad - D_{+B} D_{-B} A_n + \frac{1}{\beta^n} (\dot{g} - \beta^A \partial_A \Gamma) \end{aligned} \quad (6.132)$$

$$\begin{aligned} \dot{E}_B &\doteq \beta^n D_{-n} E_B - \frac{2}{h} \left[-D_{-n} A_B - \frac{\kappa_v + 1}{\kappa_v - 1} E_B + \frac{f_B}{\kappa_v - 1} \right] \\ &\quad - D_{+C} D_{-C} A_B + D_{0B} \Gamma \end{aligned} \quad (6.133)$$

$$\dot{\Gamma} \doteq \dot{g}. \quad (6.134)$$

We should also note that in the KWB formulation, Γ decouples from the evolution equations, satisfying a transport equation. Elsewhere, it only appears in the evolution equation for E_n and there it can simply be thought of as a forcing term because E_n does not couple back to the evolution of Γ . Hence, whatever data is given to the incoming Γ will enter the grid, be transported along the grid and then leave the grid, influencing the solution only through the evolution equation for E_n .

6.3.3 CPBC for the KWB system with shift

For the implementation of constraint preserving boundary conditions, we require the evolution of the auxiliary variable X on the boundary. The calculation runs through in a similar way as for the zero shift case; taking the standard homogeneous maximally dissipative condition on the characteristic constraint variables

$$C_+ - \kappa_c C_- = 0 \quad (6.135)$$

and substituting in the definitions

$$C_{\pm} = \partial_n U_{\pm} + \partial^A U_{\pm A}, \quad (6.136)$$

gives

$$\partial_n U_+ + \partial^B U_{+B} - \kappa_c (\partial_n U_- + \partial^B U_{-B}) = 0. \quad (6.137)$$

The evolution equations for the characteristic variables

$$\dot{U}_{\pm} = (\beta^n \pm 1) U_{\pm, n} + \beta^A U_{\pm, A} \mp A_{n, BB}, \quad (6.138)$$

give, with $\kappa_s = \kappa_c \frac{\beta^n + 1}{\beta^n - 1}$,

$$\begin{aligned} \partial_t (U_+ - \kappa_s U_-) &= -A_{n, BB} (1 + \kappa_s) - (\beta^n + 1) (U_{+B, B} - \kappa_c U_{-B, B}) \\ &\quad + \beta^A U_{+, A} - \kappa_s \beta^A U_{-, A}. \end{aligned} \quad (6.139)$$

We let

$$X = U_+ - \kappa_s U_- \quad (6.140)$$

and therefore

$$\dot{X} = \beta^A X_{,A} - A_{n,BB} \left(1 + \kappa_c \frac{\beta + 1}{\beta - 1} \right) - (\beta + 1) \partial^B \left[2 \frac{\kappa_v - \kappa_c}{\kappa_v - 1} E_B + \frac{\kappa_c - 1}{\kappa_v - 1} f_B \right], \quad (6.141)$$

where

$$U_{+B} = \kappa_v U_{-B} + f_B. \quad (6.142)$$

This means X can be used as the free data for the remaining MDBC

$$U_+ = \kappa_s U_- + f, \quad (6.143)$$

with

$$f = X. \quad (6.144)$$

Note that the relation

$$\kappa_s = \kappa_c \frac{\beta + 1}{\beta - 1} \quad (6.145)$$

means that there is a tighter restriction on κ_s .

6.3.4 The second order in space wave equation with shift

We want to be able to show well-posedness with MDBC and CPBC included and we can try to use the same approach to find an energy estimate for KWB. First we consider the shifted wave equation as a precursor to looking at an adapted energy and characteristic variables for KWB. First we outline the problem with non-zero shift for the wave equation.

Consider the standard characteristic variables for the wave equation

$$U_{\pm} = \pi \pm \partial_n \phi \quad (6.146)$$

$$U_A = \partial_A \phi \quad (6.147)$$

and the standard energy

$$\epsilon = \pi + \partial_i \phi \partial^i \phi, \quad (6.148)$$

which can be written in terms of characteristic variables as

$$\epsilon = \frac{1}{2} (U_+^2 + U_-^2) + U_A U^A, \quad (6.149)$$

with the flux

$$F^i = 2\pi\partial^i\phi \quad (6.150)$$

which in the direction n_i and written in terms of characteristic variables is

$$F^n = \frac{1}{2}(U_+^2 - U_-^2), \quad (6.151)$$

so the usual method can be used to write the integral of the energy density as a divergence of the flux which can be made non-positive or bounded by using the homogeneous or inhomogeneous MDBC respectively. Now by considering a non-zero shift, each term will obtain an extra divergence because the energy is quadratic in the variables, so for each term Y ,

$$\dot{Y} = \beta^i\partial_i Y + \text{original terms}, \quad (6.152)$$

meaning that the characteristic variables will be the same but with different speeds and the flux will become

$$F^n = \frac{1}{2}(U_+^2 - U_-^2) + \beta^n\epsilon. \quad (6.153)$$

Now, using the MDBC as above, the first term will be controlled but there is no guarantee that the second term will be controlled unless β^n is negative. If this is the case, as the energy ϵ is positive definite, the whole expression will still be bounded. However, with $\beta^n > 0$, the second term cannot be bounded using the same MDBC and a change has to be made to these boundary conditions. It is important to note that U_A is no longer implicitly a zero-speed variable, meaning that it may need a boundary condition imposed upon it. However, if we consider the evolution equation of this characteristic variable

$$\begin{aligned} \dot{U}_A &= \partial_A \dot{\phi} \\ &= \partial_A(\beta^j\partial_j\phi + \pi) \\ &= \beta^n\partial_A\partial_n\phi + \beta^B\partial_A\partial_B\phi + \partial_A\pi \\ &= \frac{1}{2}a\beta^n\partial_A(U_+ - U_-) + (1-a)\beta^n\partial_n U_A + \beta^B\partial_A\partial_B\phi + \frac{1}{2}\partial_A(U_+ + U_-), \end{aligned} \quad (6.154)$$

where a parameterizes the two different ways of writing the mixed derivative of ϕ , then setting $a = 1$ retains the zero-speed status and therefore U_A needs no additional boundary condition.

It remains to consider the problem of the uncontrolled flux

$$F^n = \frac{1}{2}(U_+^2 - U_-^2) + \beta^n\epsilon. \quad (6.155)$$

This can be dealt with by introducing an extra term and arbitrary vector field b^i into the energy itself, i.e.

$$\epsilon = \pi^2 + \partial^i \phi \partial_i \phi + 2\pi b^i \partial_i \phi. \quad (6.156)$$

Here we have simply added a term that is conserved when considering an infinite domain. Interestingly however, this term can be derived by making a first order reduction of the system, where the vector field b^i would be a field parametrising the addition of the constraint $d_{ij} - d_{ji}$ to the evolution equation of A_i . This would therefore become incorporated into the general conserved energy. When translating back to second order in space form, b^i would disappear from the evolution equation but would remain in the energy, matching the term in expression (6.156).

With the usual characteristic variables, we cannot construct this adapted energy in a simple way. Notice that

$$\frac{1}{2}(U_+^2 + U_-^2) = \pi^2 + (\partial_n \phi)^2 \quad (6.157)$$

and

$$\frac{1}{2}b_n(U_+^2 - U_-^2) = 2\pi b_n \partial_n \phi, \quad (6.158)$$

so we are left needing

$$(\partial_A \phi)^2 + 2\pi b^A \partial_A \phi, \quad (6.159)$$

which would require terms combining U_\pm and U_A , terms that would be very difficult to bound. The obvious solution is to adapt the characteristic variables by adding multiples of the transverse derivatives so that the energy can be written in a simpler form. Therefore let

$$\tilde{U}_\pm = \pi \pm \partial_n \phi + m_\pm U_A. \quad (6.160)$$

Note that it was shown above that U_A was a zero-speed characteristic variable and it can therefore be added to U_\pm without changing the character of U_\pm . So now

$$\begin{aligned} \frac{1}{2}[(1 + \beta_n)\tilde{U}_+^2 + (1 - \beta_n)\tilde{U}_-^2] &= \pi^2 + (\partial_n \phi)^2 + 2\pi b_n \partial_n \phi + \frac{1}{2}(\partial_A \phi)^2(m_+^2(1 + b_n) \\ &\quad + m_-^2(1 - b_n)) + \pi \partial_A \phi [m_+(1 + b_n) + m_-(1 - b_n)] \\ &\quad + \partial_n \phi \partial_A \phi [m_+(1 + b_n) - m_-(1 - b_n)], \end{aligned} \quad (6.161)$$

which means that we need m_\pm to satisfy

$$\frac{1}{2}(m_+(1 + b_n) - m_-(1 - b_n)) = 0 \quad (6.162)$$

$$\frac{1}{2}(m_+(1 + b_n) + m_-(1 - b_n)) = b^A, \quad (6.163)$$

for which the solution is

$$m_{\pm} = \frac{b^A}{1 \pm b_n} \quad (6.164)$$

and hence

$$\tilde{U}_{\pm} = \pi \pm \partial_n \phi + \frac{b^A}{1 \pm b_n} U_A. \quad (6.165)$$

Now

$$\frac{1}{2}[(1 + \beta_n)\tilde{U}_+^2 + (1 - \beta_n)\tilde{U}_-^2] = \pi^2 + (\partial_n \phi)^2 + 2\pi b^i \partial_i \phi + \frac{(b^A U_A)^2}{1 - b_n^2}. \quad (6.166)$$

Therefore

$$\epsilon = \frac{1}{2}[(1 + \beta_n)\tilde{U}_+^2 + (1 - \beta_n)\tilde{U}_-^2] + \left(\gamma^{ab} - \frac{b^A b^B}{1 - b_n^2} \right) U_A U_B. \quad (6.167)$$

The adapted characteristic variables change the time derivative of U_A to

$$\dot{U}_A = \beta^n \partial_A (\tilde{U}_+ - \tilde{U}_-) + \beta^B \partial_B U_A + \frac{1}{2} \partial_A (\tilde{U}_+ + \tilde{U}_-) - \frac{b^B}{1 - b_n^2} \partial_A U_B \quad (6.168)$$

and the derivatives of the characteristic variables themselves are

$$\dot{\tilde{U}}_{\pm} = \beta^i \partial_i \tilde{U}_{\pm} \pm \partial_n \tilde{U}_{\pm} + \partial^B U_B + \frac{b^A}{1 \pm b_n} \partial_A \tilde{U}_{\mp} - \left(\frac{b^A U_A}{1 \pm b_n} \right)^2. \quad (6.169)$$

Now, we calculate the flux in terms of characteristic variables. The energy is

$$\epsilon = \pi^2 + \partial^i \phi \partial_i \phi + 2\pi b^i \partial_i \phi, \quad (6.170)$$

so the time derivative is

$$\begin{aligned} \dot{\epsilon} &= \beta^i \epsilon_{,i} + 2\pi \phi_{,jj} + 2\phi_{,i} \pi_{,i} + 2\phi_{,jj} b^i \phi_{,i} + 2\pi b^i \pi_{,i} \\ &= \beta^i \epsilon_{,i} + 2(\pi \phi_{,i})_{,i} + 2b^i (\phi_{,j} \phi_{,i})_{,j} - b^j (\phi_{,i})_{,j}^2 + b^i (\pi^2)_{,i} \\ &= [\beta^j \epsilon + 2\pi \phi_{,j} + 2b^i \phi_{,j} \phi_{,i} - b^j \phi_{,i} \phi_{,i} + b^j \pi^2]_{,j}, \end{aligned} \quad (6.171)$$

which is a total divergence and hence we give the normal flux, where we now set $b^A = 0$. Note that with $b^A = 0$, $\tilde{U}_{\pm} = U_{\pm}$ so we will drop the tilde.

$$\begin{aligned} F^n &= \beta^n \epsilon + 2\pi \phi_{,j}^n + b^n \pi^2 + 2b^i \phi_{,j}^n \phi_{,i} - b^n \phi_{,i} \phi_{,i} \\ &= \beta^n \epsilon + \frac{1}{2}(U_+^2 - U_-^2) + \frac{1}{2}b^n(U_+^2 + U_-^2) - b^n U_A U^A \\ &= \frac{1}{2}[(1 + \beta^n)(1 + b^n)U_+^2 - (1 - \beta^n)(1 - b^n)U_-^2 + (\beta^n - b^n)U_A U^A]. \end{aligned} \quad (6.172)$$

Now if we set $b^n = \beta^n$, then

$$F^n = \frac{1}{2}(1 + \beta^n)^2 U_+^2 - \frac{1}{2}(1 - \beta^n)^2 U_-^2. \quad (6.173)$$

So, applying the standard MDBC

$$U_+ = \kappa U_- + f, \quad (6.174)$$

we obtain

$$F^n = \frac{1}{2}(1 + \beta^n)^2 \left[\left(\kappa^2 - \left(\frac{1 - \beta^n}{1 + \beta^n} \right)^2 \right) U_-^2 + 2\kappa U_- f + f^2 \right]. \quad (6.175)$$

So F^n is bounded if

$$|\kappa| \leq \left(\frac{1 - \beta^n}{1 + \beta^n} \right). \quad (6.176)$$

Also note that with $b^A = 0$ and $b^n = \beta^n$ it is clear that the energy is positive definite

$$\epsilon = \frac{1}{2}[(1 + \beta^n)U_+^2 + (1 - \beta^n)U_-^2]. \quad (6.177)$$

6.3.5 Constructing an energy for the KWB system with shift

When $\beta^n < 0$ we consider the energy

$$\epsilon = E_i^2 + A_{i,j}^2 - 2A_{i,i}\Gamma + \sigma\Gamma^2, \quad (6.178)$$

which we know can be controlled with MDBC without a shift. The flux will be

$$F^n = \beta^n \epsilon + U_{+i}^2 - U_{-i}^2, \quad (6.179)$$

$U_{+i}^2 - U_{-i}^2$ is bounded due to MDBC and $\beta^n \epsilon$ is negative by assumption, so the energy is bounded as required.

With $\beta^n > 0$, Γ becomes an incoming characteristic variable with the evolution equation

$$\dot{\Gamma} = \beta^j \Gamma_{,j}. \quad (6.180)$$

Unfortunately, the same technique that worked for the shifted wave equation does not work for KWB. We introduce an additional term into the energy as before

$$\epsilon = E_i^2 + A_{i,j}^2 - 2A_{i,i}\Gamma + \sigma\Gamma^2 - 2b^i E_j A_{j,i} + 2b^i E_i \Gamma, \quad (6.181)$$

so that with $b^A = 0$ we have a positive definite energy

$$\frac{1}{2}[(1 + b^n)U_{+i}^2 + (1 - b^n)U_{-i}^2] + A_{i,B}^2 - 2A_{B,B}\Gamma + (\sigma - 1)\Gamma^2 \quad (6.182)$$

and we take the time derivative to give

$$\begin{aligned} \dot{\epsilon} &= \beta^i \epsilon_{,i} + 2E_i(-A_{i,jj} + \Gamma_{,i}) - 2A_{i,j}E_{i,j} + 2E_{i,i}\Gamma \\ &\quad + 2b^i [E_j E_{j,i} - 2A_{j,i}(-A_{j,kk} + \Gamma_{,j}) + 2\Gamma(-A_{i,jj} + \Gamma_{,i})] \\ &= \left[\beta^j \epsilon - 2E_i A_{i,j} + 2E_j \Gamma + b^j E_i^2 + b^j \Gamma^2 + 2b^i A_{k,i} A_{k,j} - b^j A_{k,i}^2 \right. \\ &\quad \left. - 2b^i A_{j,i} \Gamma + 2b^j A_{i,i} \Gamma - 2b^i A_{i,j} \Gamma \right]_{,j} - 2b^i A_{j,j} \Gamma_{,i} + 2b^i A_{i,j} \Gamma_{,j}, \end{aligned} \quad (6.183)$$

so we have

$$\dot{\epsilon} = \partial_j F^j + s, \quad (6.184)$$

where, with $b^A = 0$,

$$s = -2b^i A_{j,j} \Gamma_{,i} + 2b^i A_{i,j} \Gamma_{,j} \quad (6.185)$$

and

$$F^n = \beta^n \epsilon - 2E_i A_{i,n} + 2E_n \Gamma + b^n [E_i^2 + \Gamma^2 + A_{k,n}^2 - A_{k,B}^2 - 2A_{n,n} \Gamma + 2A_{B,B} \Gamma]. \quad (6.186)$$

So, again setting $\beta^n = b^n$, we would have

$$\begin{aligned} F^n &= \beta^n \left(\frac{1}{2}[(1 + \beta^n)U_{+i}^2 + (1 - \beta^n)U_{-i}^2] + A_{i,B}^2 - 2A_{B,B}\Gamma + (\sigma - 1)\Gamma^2 \right) \\ &\quad + \frac{1}{2}(U_{+i}^2 - U_{-i}^2) + \beta^n \left(\frac{1}{2}(U_{+i}^2 + U_{-i}^2) - A_{i,B}^2 + 2A_{B,B}\Gamma \right) \\ &= \frac{1}{2} \left((1 + \beta^n)^2 U_{+i}^2 - (1 - \beta^n)^2 U_{-i}^2 \right) + \beta^n (\sigma - 1) \Gamma^2, \end{aligned} \quad (6.187)$$

which would be bounded by MDBC (including setting $\Gamma = g$ where g is free data).

However, we cannot avoid the fact that we have the source terms

$$s = -2b^n A_{B,B} \Gamma_{,n} + 2b^n A_{n,B} \Gamma_{,B}. \quad (6.188)$$

Hence it does not seem that we will be able to analytically bound the energy in this way.

We will instead look at how KWB performs empirically with MDBC.

6.4 KWB numerical results

6.4.1 KWB experimental setup

We are using the Cactus architecture for experimentation on KWB and Z1. Cactus is an “open source problem solving environment designed for scientists and engineers”, [16] which provides standard code such as grid construction, input/output routines and time-integrators for which we have written independent KWB and Z1 routines. We perform 1D and 2D tests, where the grid is 3D but the number of gridpoints in the transverse directions is reduced to a minimum. That is, for 1D tests the y and z directions are suppressed whilst for 2D tests just the z direction is suppressed. The number of points in the x direction is 20, 40, 80, 160 for the four resolutions used in these tests, doubling each time to allow simple calculation of convergence. We always use periodic boundary conditions in the y and z directions and $-0.5 \leq x \leq 0.5$ for all resolutions.

6.4.2 Stability tests

We need to test stability of the evolution code and the boundary code. The tests of the evolution code were made using periodic boundary conditions in all directions. We consider the relative energy, which is the energy at time t divided by the energy of the initial data. Figure 6.1 shows the relative energy with periodic boundary conditions and varying Courant factor λ , which is equal to the timestep divided by the spatial step, $\lambda = dt/h$. The discrete energy used

$$2E_D = \|E_i\|^2 + \|D_{+j}A_i\|^2 - 2(D_{0i}A_i, \Gamma) + \sigma\Gamma^2, \quad (6.189)$$

should be conserved. Some dissipation of the numerical solution can be seen in the figure, caused by the time integrator. However, the dissipation rate is less as the Courant factor is decreased whilst keeping the spatial resolution fixed. The limit of this behaviour as the Courant factor tends to zero is the semidiscrete result, i.e. a conserved energy. The effect of the spatial differencing can be seen in figure 6.2. Again, there is less dissipation as the spatial resolution increases tending toward a constant relative energy. In comparison, consider the altered l_2 norm $\|u\|$ where $\|u\|^2 = E_i^2 + A_i^2 + \Gamma^2 + (D_{+j}A_i)^2$. Figure 6.3 shows that $\|u\|$ is not conserved but can be bounded as

$$\|u(t)\| \leq K\|u(0)\| \quad (6.190)$$

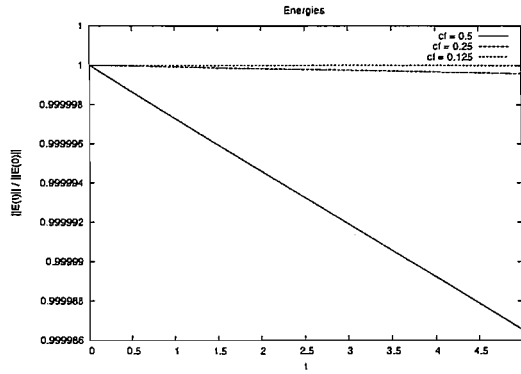


Figure 6.1: Relative energy with periodic boundary conditions and periodic initial data with various Courant factors.

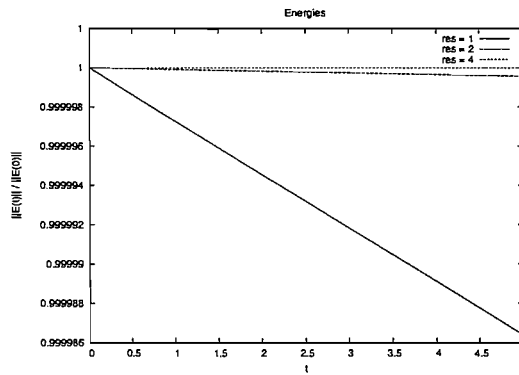


Figure 6.2: Relative energy with periodic boundary conditions and periodic initial data at various spatial resolutions.

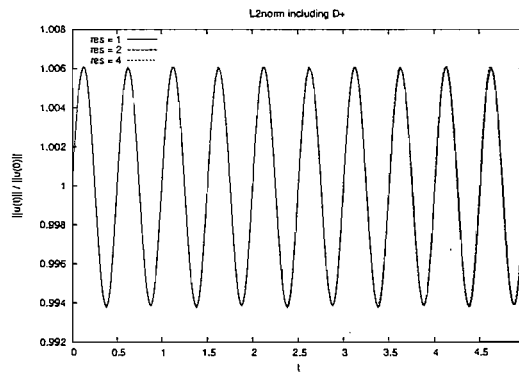


Figure 6.3: $\|u(t)\|/\|u(0)\|$ with periodic boundary conditions and periodic initial data.

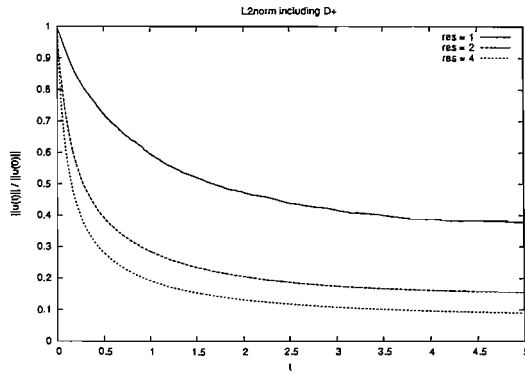


Figure 6.4: $\|u(t)\|/\|u(0)\|$ with maximally dissipative boundary conditions and noise initial data at various spatial resolutions.

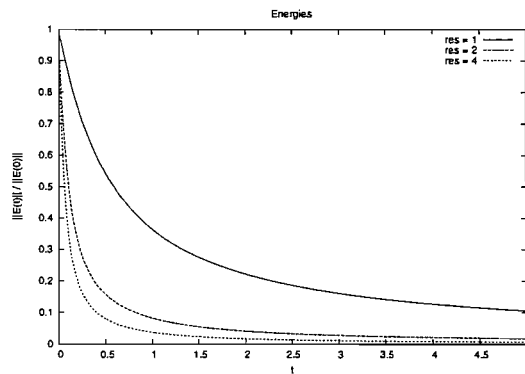


Figure 6.5: Relative conserved energy with maximally dissipative boundary conditions and noise initial data at various spatial resolutions.

with $K \approx 1.006$. The same tests can be done with maximally dissipative boundary conditions imposed. In addition, arbitrary free data can be used at the boundaries. We test the stability of the code with artificial boundaries by (i) setting the free data at the boundaries to zero and using random noise initial data and (ii) by using zero initial data and non-zero free boundary data; in this case the free boundary data will be set to one and then turned off at a certain time, which we will call ‘top hat’ boundary data.

The same tests were done with the MDBC coupling constants set to 0 and to -1 . The two figures 6.4 and 6.5 show that $\|u\|$ and the energy are non-increasing when random noise is used as initial data. This is to be expected as the analytical time derivative of the energy is non-positive. Here there is a qualitative difference between $\|u\|$ and the energy. For strong stability, the following estimate must

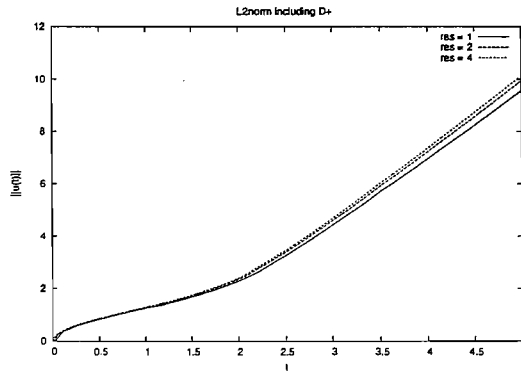


Figure 6.6: $\|u\|$ with maximally dissipative boundary conditions and zero initial data at various spatial resolutions with ‘top hat’ free boundary data. $f_n = 1$ until $t = 3.5$. MDBC coupling constants set to -1.

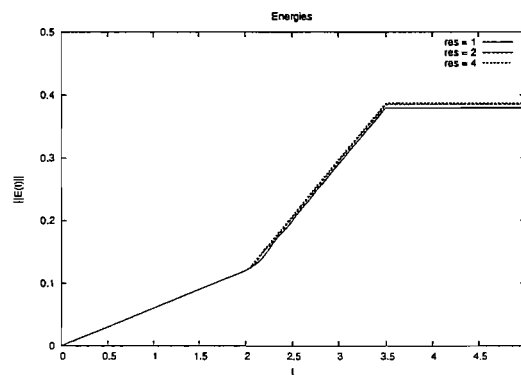


Figure 6.7: Energy with maximally dissipative boundary conditions and zero initial data at various spatial resolutions with ‘top hat’ free boundary data. $f_n = 1$ until $t = 3.5$. MDBC coupling constants set to -1.

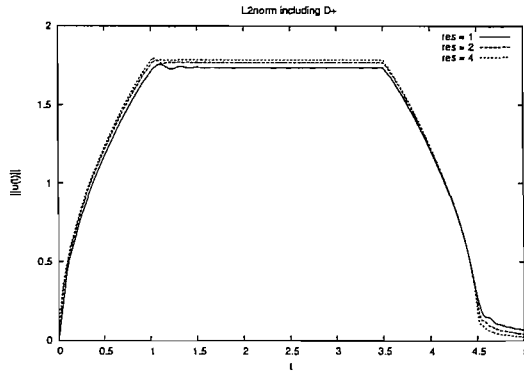


Figure 6.8: $\|u\|$ with maximally dissipative boundary conditions and zero initial data at various spatial resolutions with ‘top hat’ free boundary data. $f_n = 1$ until $t = 3.5$. MDBC coupling constants set to 0.

hold:[7]

$$\|v(t)\|_h^2 \leq K(t) \left(\|v(t_0)\|_h^2 + \max_{t_0 \leq \tau \leq t} (|f_0(\tau)|^2 + |g_N(\tau)|^2) \right). \quad (6.191)$$

With the initial data zero, this implies that the solution must satisfy

$$\|v(t)\|_h^2 \leq K(t) \max_{t_0 \leq \tau \leq t} (|f_0(\tau)|^2 + |f_N(\tau)|^2) \quad (6.192)$$

and as the maximum value of the free boundary data is in this case 1, this means the solution must be bounded by the function $K(t)$, which must be a bounded function in any finite time interval.

The energy in figure 6.7 increases while the free data is equal to one. It then increases faster when the information has been able to cross to the opposite boundary and back. At $t = 3.5$ the free data is turned off and hence the energy again becomes conserved. With $\|u\|$, figure 6.6, the amplitude keeps increasing even when the free data has been turned off. This is due to a gradual increase in A_i , a term that is present in $\|u\|$ but not present in E .

Considering the case with MDBC coupling constants set to zero, the situation is clearer. Figures 6.8 and 6.9 show that the respective norms increase as free data is added at one boundary. After $t = 1$ the free data input has propagated to the opposite boundary where it will flow out of the system. At that point the norm levels out because the injection of energy equals the loss at the opposite boundary. At $t = 3.5$, the injection of data ceases and at $t = 4.5$, the data has left the domain.

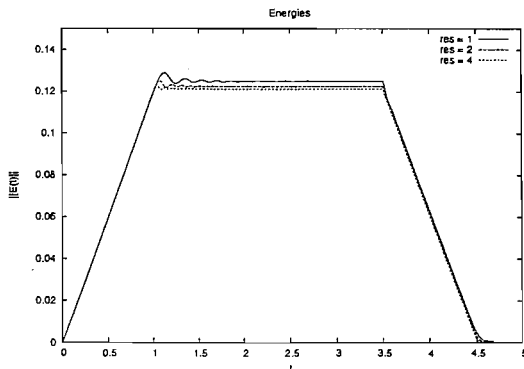


Figure 6.9: Energy with maximally dissipative boundary conditions and zero initial data at various spatial resolutions with ‘top hat’ free boundary data. $f_n = 1$ until $t = 3.5$. MDBC coupling constants set to 0.

It is noteworthy that when using the periodic exact solution given above, if the only non-zero wavenumber is k_x , then $k_x = \omega$ and to satisfy the constraints, a_x must be zero. Therefore, with the coupling constant κ_1 set to zero, the free data satisfies

$$\begin{aligned}
 f = U_+ &= -A_{n,n} + E_n + \Gamma \\
 &= -a_x k_x (\sin \omega t + \cos \omega t) \cos(k^i x_i) + \frac{k_x^2}{\omega^2} \sin(k^i x_i) \\
 &\quad + a_x \omega (\sin \omega t - \cos \omega t) \sin(k^i x_i) - \sin(k^i x_i) \\
 &= 0.
 \end{aligned} \tag{6.193}$$

Therefore, with this exact solution it will be necessary to work in 2D to give a non-zero value of f .

6.4.3 Convergence testing

The convergence plots (6.10 - 6.15) show convergence in 1D and 2D for periodic boundary conditions, MDBC and CPBC. All the errors are scaled by the expected second order convergence factor so that perfect convergence would have all curves coincident. The only subtlety here is in figure 6.15, where the errors do not decrease quite enough as the resolution increases. However, this problem also disappears as the resolution increases and is a consequence of constraint violations being expelled from the grid.

Considering the case with non-zero shift, figure 6.16 shows that we still retain convergence, even using CPBC. Note that we can still compare to the exact so-

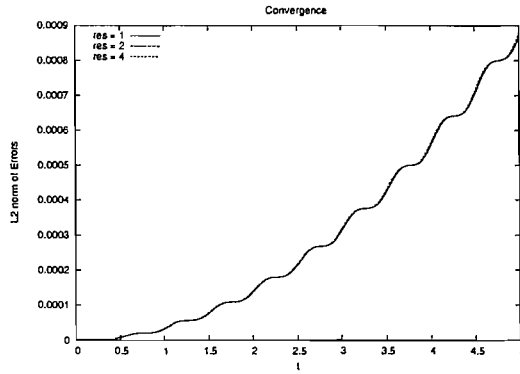


Figure 6.10: l_2 norm of the errors with periodic boundary conditions in 1D.

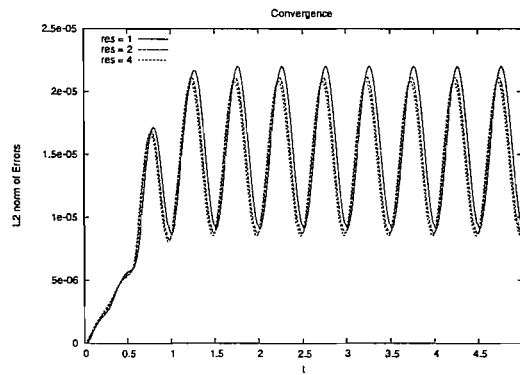


Figure 6.11: l_2 norm of the errors with maximally dissipative boundary conditions in 1D.

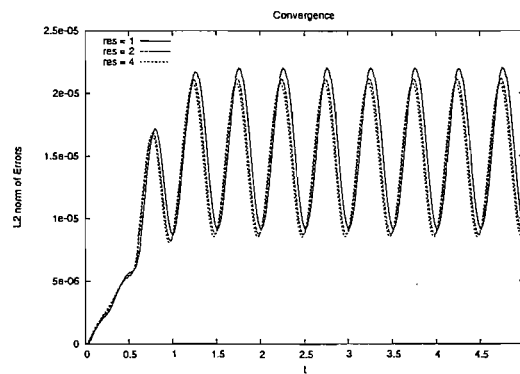


Figure 6.12: l_2 norm of the errors with constraint preserving boundary conditions in 1D.

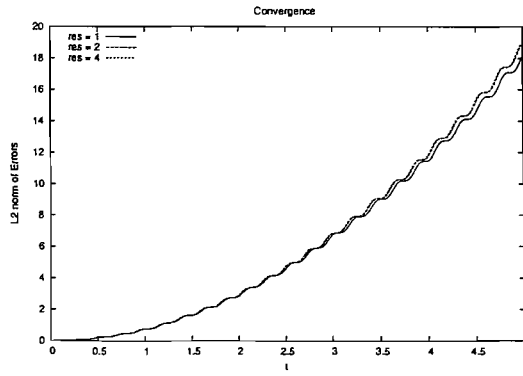


Figure 6.13: l_2 norm of the errors with periodic boundary conditions in 2D.

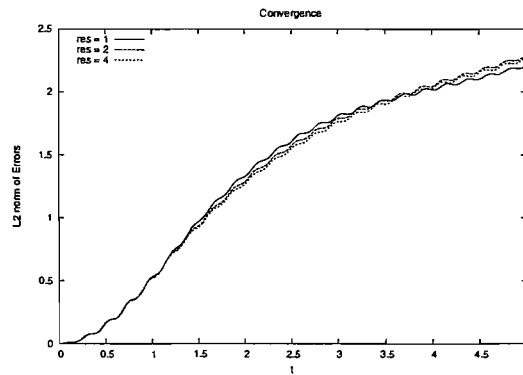


Figure 6.14: l_2 norm of the errors with maximally dissipative boundary conditions in 2D.

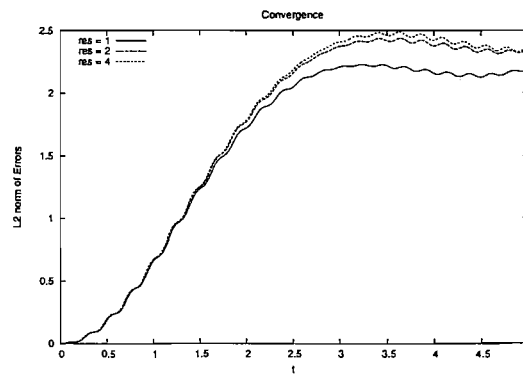


Figure 6.15: l_2 norm of the errors with constraint preserving boundary conditions in 2D.

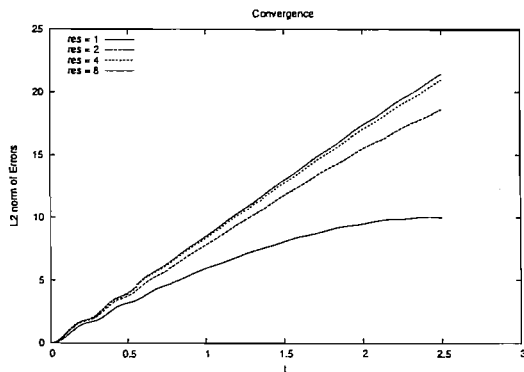


Figure 6.16: l_2 norm of the errors with constraint preserving boundary conditions in 2D with non-zero shift and exact data for incoming Γ .

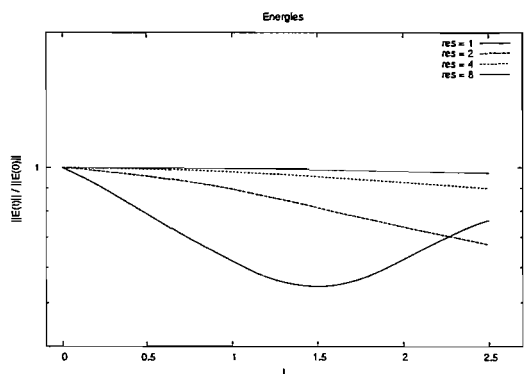


Figure 6.17: Relative Energy with constraint preserving boundary conditions in 2D with non-zero shift and exact data for incoming Γ .

lution because there was no initial constraint violation. The shift in the normal and transverse directions have been set to positive non-zero values, so that there are still the same number of incoming and outgoing characteristics except for the additional Γ (which was previously a zero-speed characteristic) for which exact data is given at the incoming boundary. The scaled errors again do not quite match up but as resolution increases this misalignment improves. In figure 6.17 the relative energy clearly tends toward unity as the resolution increases.

We return to 1D to consider the introduction of an initial constraint violation in the initial data. Figure 6.18 shows second order self-convergence in the situation without any constraint violation. With the presence of initial constraint violation, figure 6.19 shows that there is a drop of convergence as a reaction between the initial constraint violation and the left boundary as the violation propagates out of the grid. As soon as this initial feature has left the grid we regain second order

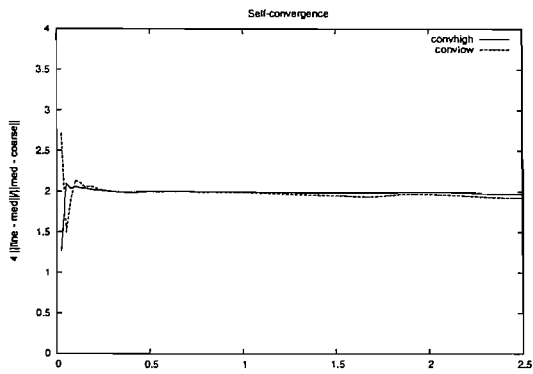


Figure 6.18: Self-convergence with CPBC with shift and no initial constraint violation in 1D.

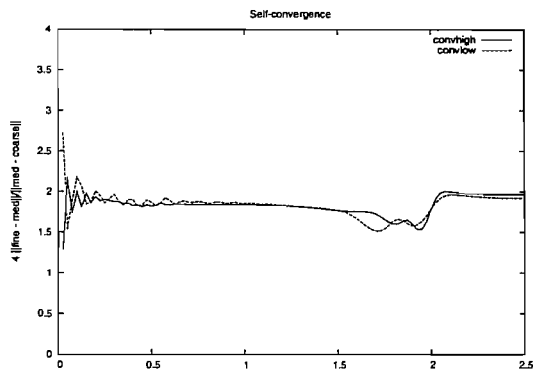


Figure 6.19: Self-convergence with CPBC with shift and initial constraint violation in 1D.

convergence.

Chapter 7

The Z1 System

7.1 Energy without boundaries

By using general quadratic forms of the evolution variables and the relationship

$$\dot{\epsilon} = \partial^i F_i + s, \quad (7.1)$$

we can give a general form for the energy density, flux and source terms [14]

$$\begin{aligned} \epsilon &= c_0[E_i^2 + A_{i,j}^2 - 2A_{j,j}(Z + A_{i,i})] \\ &\quad + c_1(Z + A_{i,i})^2 \\ &\quad + c_2(A_{i,i}^2 - A_{i,j}A_{j,i}), \end{aligned} \quad (7.2)$$

$$\begin{aligned} F_i &= 2c_0[-A_{j,i}E_j + E_i(Z + A_{j,j})] \\ &\quad + 2c_2(A_{i,j}E_j - A_{j,j}E_i), \end{aligned} \quad (7.3)$$

$$s = 2\kappa Z[(c_0 - 2c_1)A_{i,i} - 2c_1Z], \quad (7.4)$$

where c_0 , c_1 and c_2 are arbitrary constants. If we define $c \equiv c_2/c_0$, the energy is positive definite for

$$c_0 > 0, \quad -\frac{1}{2} < c < 1, \quad \frac{c_1}{c_0} > \frac{3}{1+2c}. \quad (7.5)$$

This means that with no boundaries (periodic boundary conditions) and the damping parameter κ equal to zero, we have a conserved energy at the continuum.

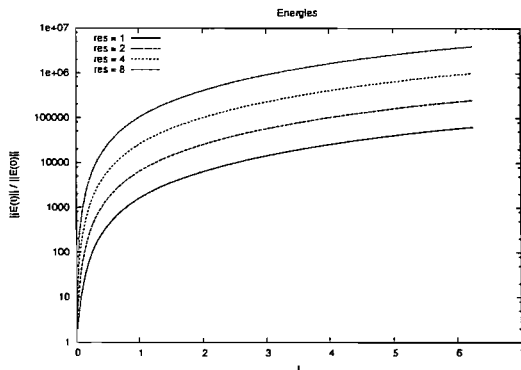


Figure 7.1: Relative energy $E(t)/E(0)$ for increasing resolution using the solution $A_1 = (-1)^i t$ and $E_1 = (-1)^{i+1}$ and no dissipation.

7.2 Discretisation of the Z1 system

Above we showed that, at the continuum level, there is a conserved energy up to boundary flux. Restricting our consideration to the case of no boundaries, we can attempt to find the corresponding discrete conserved energy. Considering the standard discretisation of the evolution equations, we have the exact solution $A_n = (-1)^i t$, $E_n = (-1)^{i+1}$ with all other variables zero. The continuum energy density

$$\epsilon = E_i^2 + A_{i,j}^2 - 2A_{i,i}\Gamma + \sigma\Gamma^2, \quad (7.6)$$

has two basic choices for the discretisation of the continuum term $A_{i,j}$: (i) $D_{+j}A_i$ and (ii) $D_{0j}A_i$. For case (i) and the exact solution given above, the ratio of energy density at time t and initial time is

$$\frac{\epsilon(t)}{\epsilon(0)} = 1 + 4\frac{t^2}{h^2} \quad (7.7)$$

and so the relative energy density can be made arbitrarily large by increasing the resolution. The scheme is therefore unstable with respect to this energy. Testing this exact solution with periodic boundaries clearly shows the greater energy growth as the resolution is increased (figure 7.1). To prevent this instability, we can introduce some artificial dissipation into the evolution equations for all variables, i.e. terms of the form $-\sigma_d h^3 (D_+ D_-)^2$. At the limit of resolution this term will disappear due to the h^3 , however it will damp out the highest frequency modes therefore preventing the exact solution above from causing an instability.

Figures 7.2 - 7.4 show that as the value of the dissipation parameter increases, the energy of the solution is more quickly damped. This is to be expected because

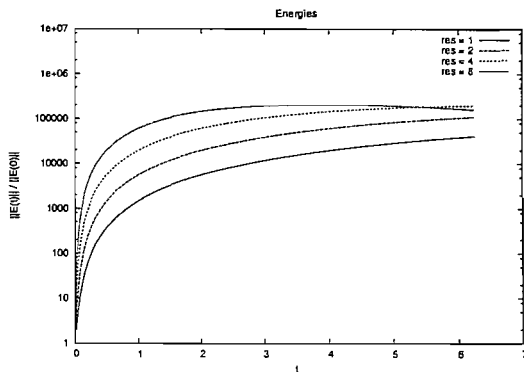


Figure 7.2: Relative energy $E(t)/E(0)$ for increasing resolution using the solution $A_1 = (-1)^i t$ and $E_1 = (-1)^{i+1}$ and dissipation $\sigma_d = 0.0001$.

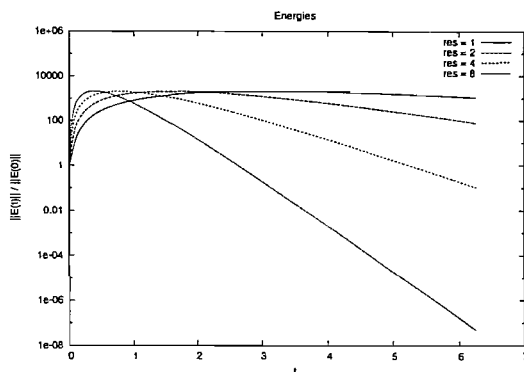


Figure 7.3: Relative energy $E(t)/E(0)$ for increasing resolution using the solution $A_1 = (-1)^i t$ and $E_1 = (-1)^{i+1}$ and dissipation $\sigma_d = 0.001$.

artificial dissipation damps high frequency modes and our initial data in this case is constructed of the highest frequency mode. After a particular time in each figure (a shorter time as σ_d increases), the relative energy is lower as resolution increases, showing that the scheme is no longer unstable. Since a larger value of σ_d means that the high frequency modes will be damped more quickly, we want σ_d as large as possible; however, there is an upper limit on the value of σ_d that is useful because too much dissipation can make the scheme unstable (see figure 7.5 with $\sigma_d = 0.35$). In conclusion, a reasonable value of dissipation to use is $\sigma_d = 0.025$ as this value is high enough to quickly dissipate any high frequency modes that have been excited whilst still being well below the value that makes the scheme unstable. This value will be used for the further work on Z1.

Note that the artificial dissipation introduced is equivalent to treating the two derivatives of $\partial^j \partial_i A_j$ and $\partial^j \partial_j A_i$ with different discretisations when $i = j$, whereas

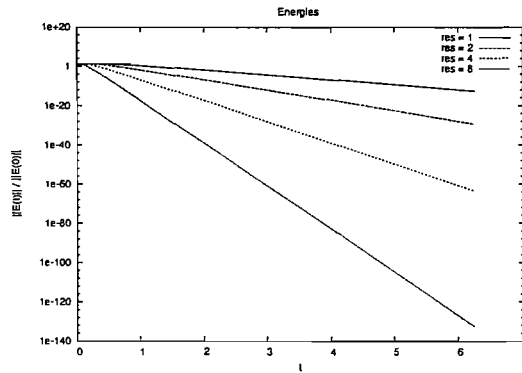


Figure 7.4: Relative energy $E(t)/E(0)$ for increasing resolution using the solution $A_1 = (-1)^i t$ and $E_1 = (-1)^{i+1}$ and dissipation $\sigma_d = 0.01$.

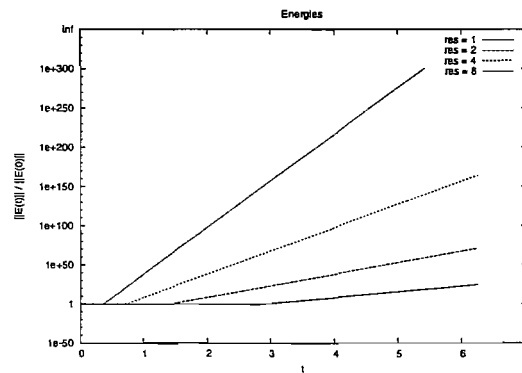


Figure 7.5: Relative energy $E(t)/E(0)$ for increasing resolution using the solution $A_1 = (-1)^i t$ and $E_1 = (-1)^{i+1}$ and dissipation $\sigma_d = 0.35$.

at the continuum these derivatives would always cancel.

For case (ii) and the exact solution $A_1 = (-1)^i$ with all other variables zero, the energy density is not positive definite and does not ‘see’ this highest frequency solution.

To use summation by parts to get a conserved energy, the approximation for the second spatial derivative of A_i in the evolution equations of E_i must match that of the approximation of $\partial_j A_i$ in the energy. For example

$$\epsilon = E_i^2 + (D_{0j}A_i)^2 - 2D_{0i}A_i\Gamma + \sigma\Gamma^2 \quad \dot{E}_i = -D_{0j}^2A_i + D_{0j}D_{0i}A_j + D_{0i}Z, \quad (7.8)$$

where D_+D_- in the evolution equations matches to D_+ or D_- in the energy, and

$$\epsilon = E_i^2 + (D_{+j}A_i)^2 - 2D_{0i}A_i\Gamma + \sigma\Gamma^2 \quad \dot{E}_i = -D_{+j}D_{-j}A_i + D_{0j}D_{0i}A_j + D_{0i}Z, \quad (7.9)$$

where D_0^2 matches to D_0 in the energy. This can be seen by using the summation by parts equations found in Appendix C. Hence we are very limited in the choice of discretisations if we wish to use this property.

7.3 Discrete boundaries for the Z1 system

We want to prescribe consistent, stable discrete boundary conditions to the Z1 system in a methodical way that can then be generalised to other systems. For the continuum, an energy was introduced in terms of characteristic variables. The energy was shown to be conserved for periodic boundary conditions bounded for maximally dissipative boundary conditions. We now want to discretise the boundary conditions and find a way to evolve all the evolution variables on the boundary. In an attempt to make our techniques methodical we will break the evolution equations into parts so we can use standard techniques and then combine these techniques to give a full prescription for the system.

7.3.1 Decomposition of the Z1 system into wave equations

Recalling the derivation of the characteristic variables for the Z1 system, we again consider only the derivatives in the direction n_i but here we take this direction

to be normal to the boundary, in the x direction. An energy can be bounded by applying maximally dissipative boundary conditions to the incoming characteristic variables. These MDBC will be used to inject information into the grid through normal derivatives. Because we know how to deal with transverse derivatives at the boundary, we will neglect these, which allows us to decompose the Z1 system of equations into groups of equations that behave as a first order wave equation (7.10 - 7.11) and a second order wave equation (7.12 - 7.13):

$$\dot{E}_n = Z_{,n} \quad (7.10)$$

$$\dot{Z} = E_{n,n} \quad (7.11)$$

$$\dot{E}_B = -A_{B,nn} \quad (7.12)$$

$$-\dot{A}_B = E_B. \quad (7.13)$$

So, first we consider maximally dissipative boundary conditions with the first order wave equation. The second order wave equation has been covered above in Section 3.2.1.

7.3.2 The first order in space wave equation

The first order wave equation in one dimension can be written

$$\dot{\phi} = \pi \quad (7.14)$$

$$\dot{\pi} = \psi' \quad (7.15)$$

$$\dot{\psi} = \pi', \quad (7.16)$$

however like $\dot{A}_i = -E_i$, ϕ can be evolved directly on the boundary so we can ignore (7.14). We discretise in the natural way with the D_0 difference operator.

$$\dot{\pi}_i = D_0\psi_i \quad (7.17)$$

$$\dot{\psi}_i = D_0\pi_i. \quad (7.18)$$

The characteristic variables are

$$U_{\pm} = \pi \pm \psi, \quad (7.19)$$

with evolution equations

$$\dot{U}_{\pm} = \pm U'_{\pm}. \quad (7.20)$$

We split the problem into the outgoing and incoming characteristics. Considering the incoming characteristic using simplified MDBC with $\kappa = 0$,

$$U_+ \doteq f. \quad (7.21)$$

Let E be the L_2 norm of U_+ on the boundary

$$E = \|U_+\|^2 = \int_{-\infty}^N U_+^2 dx. \quad (7.22)$$

Now the time derivative:

$$\dot{E} = 2 \int_{-\infty}^N U_+ \dot{U}_+ dx \quad (7.23)$$

$$= 2 \int_{-\infty}^N U_+ (U_+)' dx \quad (7.24)$$

$$= (U_+^N)^2 = f^2, \quad (7.25)$$

substituting for U_+ using (7.21).

Now we look at the discretisation of the continuum energy, taking the scalar product as a sum over $j = N - 1, N - 2, N - 3, \dots$

$$W = h \|U_{+i}\|^2 + \frac{h}{2} (U_+^N)^2, \quad (7.26)$$

where the factor of a half comes from the fact that the energy must be consistent when joining two domains together.

The time derivative of the energy is

$$\dot{W} = 2h(U_{+i}, D_0 U_{+i}) + hU_+^N \dot{U}_+^N \quad (7.27)$$

$$= U_+^N U_+^{N-1} + hU_+^N \dot{U}_+^N \quad (7.28)$$

$$= fU_+^{N-1} + hf\dot{U}_+^N, \quad (7.29)$$

using summation by parts again and substituting $U_+^N = f$.

We want the time derivative of the discrete energy (7.29) to be equal to the time derivative of the continuum energy (7.25) and so we set

$$fU_+^{N-1} + hf\dot{U}_+^N = f^2, \quad (7.30)$$

which can be rearranged to give

$$\dot{U}_+^N = \frac{1}{h}(f - U_+^{N-1}). \quad (7.31)$$

This is a nice expression as it can be written as a one-sided derivative plus a penalty term:

$$\dot{U}_+^N = \frac{1}{h}(f - U_+^N + U_+^N - U_+^{N-1}) = D_- U_+^N + \frac{1}{h}(f - U_+^N). \quad (7.32)$$

Penalty terms act like constraints and can be added to evolution equations with the correct sign to force the solution toward the ‘constraint surface’.

Now considering the outgoing characteristic variable, we let $E = \|U_-\|^2$ and hence

$$\dot{E} = -(U_-^N)^2. \quad (7.33)$$

To attain consistency we need the discrete energy, to be equivalent to the continuum, which means

$$-(U_-^N)^2 = -U_-^N U_-^{N-1} + h U_-^N \dot{U}_-^N \quad (7.34)$$

and hence

$$\dot{U}_-^N = \frac{1}{h}(U_-^{N-1} - U_-^N) = -D_- U_-^N. \quad (7.35)$$

Rewriting π^N and ψ^N in terms of the ingoing and outgoing characteristic variables and substituting in equations (7.32) and (7.35) then gives the full system in terms of evolution variables:

$$\begin{cases} \dot{\pi}_i = D_0 \psi_i \\ \dot{\psi}_i = D_0 \pi_i \end{cases} \quad i > 0$$

$$\dot{\pi}^N = \frac{1}{2}(\dot{U}_+^N + \dot{U}_-^N) \quad (7.36)$$

$$= \frac{1}{2}\left(D_-(U_-)^N + \frac{1}{h}(f - (U_+)^N) - D_-(U_-)^N\right) \quad (7.37)$$

$$= D_- \psi^N + \frac{1}{2h}(f - \pi^N - \psi^N) \quad (7.38)$$

$$\dot{\psi}^N = \frac{1}{2}(\dot{U}_+ - \dot{U}_-) \quad (7.39)$$

$$= \frac{1}{2}\left(D_-(U_+)^N + \frac{1}{h}(f - (U_+)^N) + D_-(U_-)^N\right) \quad (7.40)$$

$$= D_- \pi^N + \frac{1}{2h}(f - \pi^N - \psi^N). \quad (7.41)$$

This derivation is done as an example of a prescription for the boundaries that we will use. The more general cases for the boundary prescriptions we will implement will be of two forms. For type-1, we will set the penalty term for outgoing variables to zero and add a parameter τ to the penalty term for incoming variables

$$\dot{U}_+^N = D_- U_+^N - \frac{\tau}{h} P \quad (7.42)$$

$$\dot{U}_-^N = -D_- U_-^N, \quad (7.43)$$

where

$$P = (U_+^N - \kappa U_-^N - f) \quad (7.44)$$

and

$$\dot{U}_+^N = +D_- U_+^N - \tau Q \quad (7.45)$$

$$\dot{U}_-^N = -D_- U_-^N, \quad (7.46)$$

where

$$Q = (D_- U_+^N + \kappa D_- U_-^N - \dot{f}). \quad (7.47)$$

The prescription derived above matches to (7.42) with $\tau = 1$ and $\kappa = 0$. These two general prescriptions (7.42) and (7.45) will be called P-class and Q-class respectively. Written in this form, it can be seen that they are constructed of one-sided derivatives and penalty terms at the boundary, where the penalty terms are proportional to the maximally dissipative boundary condition for the P-class and the time derivative of this condition for the Q-class.

Type-2 boundaries will be constructed to put a bound on the energy. This is done by considering the standard discrete energy

$$E = h(\|U_+\|^2 + \|U_-\|^2) + \frac{h}{2}((U_+^N)^2 + (U_-^N)^2), \quad (7.48)$$

which we differentiate to give

$$\dot{E} = (U_+^N)^2 - (U_-^N)^2 - h(U_+^N D_+ U_+^N - U_-^N D_+ U_-^N) + h(U_+^N \dot{U}_+^N + U_-^N \dot{U}_-^N). \quad (7.49)$$

Substituting in (7.42) gives

$$\dot{E} = (U_+^N)^2 - (U_-^N)^2 + [\tau_1 U_+^N + \tau_2 U_-^N]P, \quad (7.50)$$

whilst substituting in (7.45) gives

$$\dot{E} = (U_+^N)^2 - (U_-^N)^2 + h[\tau_1 U_+^N + \tau_2 U_-^N]Q. \quad (7.51)$$

We can bound the energy by ensuring that the term in square brackets multiplied by the penalty term is a non-positive square. Therefore, we set

$$\tau_1 = -\frac{\tau}{1 + \kappa^2} \quad (7.52)$$

and

$$\tau_2 = \frac{\kappa\tau}{1 + \kappa^2}, \quad (7.53)$$

where τ is a positive constant. This gives evolution equations for the characteristic variables

$$\dot{U}_+^N = D_- U_+^N - \frac{\tau}{1 + \kappa^2} P \quad (7.54)$$

$$\dot{U}_-^N = -D_- U_-^N + \frac{\kappa\tau}{1 + \kappa^2} P \quad (7.55)$$

and the time derivative of the energy

$$\dot{\epsilon} = (U_+^N)^2 - (U_-^N)^2 - \frac{\tau}{1 + \kappa^2} (U_+^N - \kappa U_-^N) P, \quad (7.56)$$

which is non-positive for $f = 0$. With $f \neq 0$, the energy will be bounded by a function of f .

For Q-class, the process is very similar. With the same definitions of τ_1 and τ_2 , we obtain evolution equations for the characteristic variables

$$\dot{U}_+^N = D_- U_+^N - \frac{h\tau}{1 + \kappa^2} Q \quad (7.57)$$

$$\dot{U}_-^N = -D_- U_-^N + \frac{h\kappa\tau}{1 + \kappa^2} Q \quad (7.58)$$

and the time derivative of the energy

$$\dot{\epsilon} = (U_+^N)^2 - (U_-^N)^2 - \frac{h\tau}{1 + \kappa^2} (U_+^N - \kappa U_-^N) Q, \quad (7.59)$$

which is again non-positive for $f = 0$.

7.3.3 Numerical results for the first order wave equation

First considering the P1 prescription, a negative value of τ gives the wrong sign for the penalty term. For example, an increase in U_+ would result in an increase of \dot{U}_+ rather than the required decrease. The numerical results verify this by showing a blow-up of the norm. For $0 < \tau < 1$, second order convergence is lost at late times, shown in figure 7.6.¹ This situation improves when $\tau > 1$, shown in figure 7.7. As the value of τ becomes larger, the Courant factor has to be reduced to retain stability.

For P2, τ must be positive. For $\kappa = 0$ this reduces down to the P1 form but for all κ the same kind of instability occurs as for P1 as τ increases; the Courant factor has to be decreased as τ grows to much greater than 1. Until this point is reached, the solution is second order convergent, for example figure 7.8. For Q1,

¹Note the parameter a on some figures satisfies $a = -\frac{1}{4}\tau$

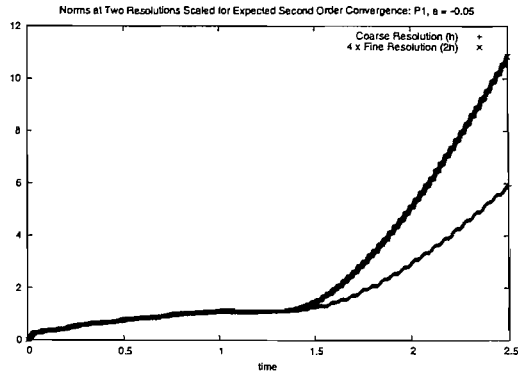


Figure 7.6: l_2 norm for coarse resolution and fine resolution, with fine norm scaled by four to show loss of second order convergence: P1 $\tau = 0.2$.

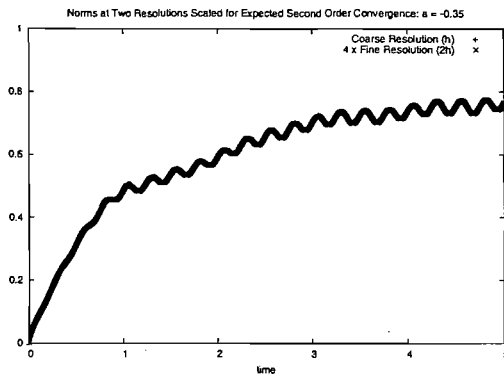


Figure 7.7: l_2 norm for coarse resolution and fine resolution, with fine norm scaled by four to show second order convergence: P1 $\tau = 1.4$.

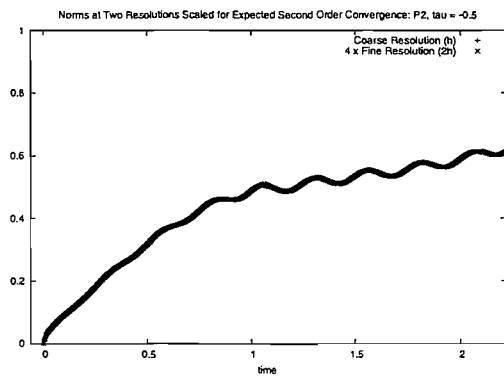


Figure 7.8: l_2 norm for coarse resolution and fine resolution, with fine norm scaled by four to show second order convergence: P2 $\tau = 0.5$.

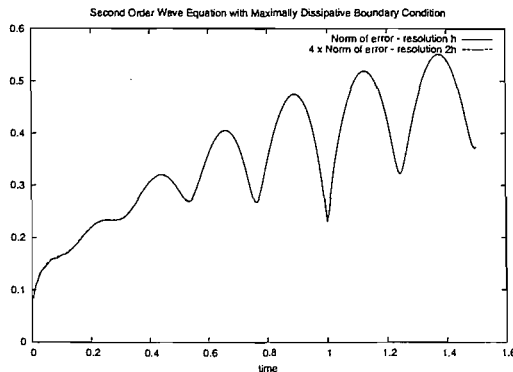


Figure 7.9: l_2 norm of the error in π and $D_+\phi$ at coarse and fine resolution for the second order wave equation using maximally dissipative boundary conditions. Norm of fine resolution is scaled to show second order convergence.

τ must again be positive, but the only value that gives second order convergence is $\tau = 1$. Q2 is also second order convergent for $\tau = 1$.

There seems little difference between the different prescriptions here, however it is important to note that Q-type only allows $\tau = 1$. P2 and Q2 seem to be preferable conceptually because the inherent bound on the energy may prove to be useful.

7.3.4 The second order in space wave equation

We implemented the second order wave equation with maximally dissipative boundary conditions using the prescription given in Section 3.2.1 and obtained second order convergence. In figure 7.9 we show the norm of the error in π and $D_+\phi$ with the norm scaled by a factor of 4 to show second order convergence. We have automatic second order convergence for all cases except when the coupling constant κ of the maximally dissipative boundary conditions is positive, in which case we have to decrease the time step as the magnitude of κ increases; for example, with a Courant factor of 0.25, $\kappa = 0.5$ gives an instability. We believe this instability is related to the integration over the time step, however we will initially be concentrating on the case where $\kappa = 0$, so this will not cause a problem.

7.4 Semi-discrete boundary conditions for the Z1 system

The next step is to put together the methods for finding boundary conditions for the first order wave equation and the second order wave equation to form a consistent, stable boundary prescription for the Z1 system. It would seem that there are enough conditions to evolve all the variables on the boundaries - four using the second order technique and two using the first order technique plus the additional evolution equations for A_i that requires no derivatives. When the shift is non-zero, exact data will be given to A_1 at one boundary and the remaining ghost points will be populated using extrapolation. Here we use the coding notation of subscript 1 representing n .

We showed in Section 7.2 that the Z1 evolution code could be made stable with the use of a small amount of artificial dissipation. Now we show the results with boundaries added.

We are using the second-order wave equation prescription for the variables A_2 and A_3 . By setting A_1 , E_1 and Z to zero in the initial data, the solution was shown to be second order convergent in these variables. With no shift, we use extrapolation for A_1 . However, with shift, we can specify $A_{1,1}$ by using the incoming characteristic variable $U_0 = Z + A_{1,1}$ and hence we can populate the ghost point for A_1 . We use the first order wave equation method for E_1 and Z . All remaining ghost points are populated with extrapolation. Recall the boundary conditions used for the first order wave equation, here given at the boundary $j = N$:

$$\dot{U}_+ \doteq D_- U_+ - \tau Y \quad (7.60)$$

$$\dot{U}_- \doteq -D_- U_-, \quad (7.61)$$

for P1 and Q1 and

$$\dot{U}_+ \doteq D_- U_+ - \frac{\tau}{1 + \kappa^2} Y \quad (7.62)$$

$$\dot{U}_- \doteq -D_- U_- + \frac{\tau \kappa}{1 + \kappa^2} Y, \quad (7.63)$$

for P2 and Q2, where Y is the penalty term P or hQ from Section 7.3.2.

Considering P1 with $\beta^n \neq 0$ but the transverse shifts set to zero for simplicity, the penalty term is still

$$P = U_+ - \kappa U_- - f \quad (7.64)$$

and the evolution equations of the characteristic variables

$$U_{\pm} = Z \pm E_n, \quad (7.65)$$

are

$$\dot{U}_+ = (\beta^n + 1)D_{-n}U_+ + D_{0B}E_B - D_{-B}D_{+B}A_n + D_{0B}A_{B,n} - \frac{\tau}{h}P \quad (7.66)$$

$$\dot{U}_- = (\beta^n - 1)D_{-n}U_- + D_{0B}E_B + D_{-B}D_{+B}A_n - D_{0B}A_{B,n} \quad (7.67)$$

and hence for the evolution variables

$$\dot{Z} = \beta^n D_{-n}Z + D_{-n}E_n + D_{0B}E_B - \frac{\tau}{2h}P \quad (7.68)$$

$$\dot{E}_n = \beta^n D_{-n}E_n + D_{-n}Z - D_{+B}D_{-B}A_n + D_{0B}(A_{B,n}) - \frac{\tau}{2h}P. \quad (7.69)$$

This will be exactly the same for the Q1 boundary condition, with

$$\begin{aligned} Q = & (\beta^n + 1)D_{-n}U_+ - \kappa(\beta^n - 1)D_{-n}U_- - \dot{f} + (1 - \kappa)D_{0B}E_B \\ & + (1 + \kappa)(D_{0B}A_{B,n} - D_{-B}D_{+B}A_n). \end{aligned} \quad (7.70)$$

For the P2 and Q2 specifications, the equations can be considered in much the same way as above, the only difference being a change of the coefficients so that they incorporate κ terms, i.e. for P2, we have

$$\dot{U}_+ = (\beta^n + 1)D_{-n}U_+ + D_{0B}E_B - D_{-B}D_{+B}A_n + D_{0B}A_{B,n} - \frac{\tau}{1 + \kappa^2} \frac{P}{h} \quad (7.71)$$

$$\dot{U}_- = (\beta^n - 1)D_{-n}U_- + D_{0B}E_B + D_{-B}D_{+B}A_n - D_{0B}A_{B,n} + \frac{\kappa\tau}{1 + \kappa^2} \frac{P}{h} \quad (7.72)$$

and

$$\dot{Z} = \beta^n D_{-n}Z + D_{-n}E_n + D_{0B}E_B + \frac{\tau}{2h} \frac{\kappa - 1}{1 + \kappa^2} P \quad (7.73)$$

$$\dot{E}_n = \beta^n E_{-n}E_n + D_{-n}Z - D_{+B}D_{-B}A_n + D_{0B}(A_{B,n}) - \frac{\tau}{2h} \frac{\kappa + 1}{1 + \kappa^2} P. \quad (7.74)$$

7.5 Numerical results for the Z1 system with boundaries

Beginning with P1, we populate the ghost point for E_n and Z by assuming that a second order accurate centred derivative approximation for the derivative is equal

to the one-sided derivative and penalty term from the evolution equation.

$$\beta^n D_{0n} Z + D_{0n} E_n = \beta^n D_{-n} Z + D_{-n} E_n - \frac{\tau}{2h} P \quad (7.75)$$

$$\beta^n D_{0n} E_n + D_{0n} Z = \beta^n D_{-n} E_n + D_{-n} Z - \frac{\tau}{2h} P \quad (7.76)$$

and hence by rearranging these expressions, the result is

$$E_{n(N+1)} = 2E_{n(N)} - E_{n(N-1)} - \frac{\tau P}{\beta^n + 1} \quad (7.77)$$

$$Z_{n(N+1)} = 2Z_{n(N)} - Z_{n(N-1)} - \frac{\tau P}{\beta^n + 1}. \quad (7.78)$$

Q1 will be similar, however there will be no division by h in the evolution equations so

$$E_{n(N+1)} = 2E_{n(N)} - E_{n(N-1)} - \frac{h\tau Q}{\beta^n + 1} \quad (7.79)$$

$$Z_{n(N+1)} = 2Z_{n(N)} - Z_{n(N-1)} - \frac{h\tau Q}{\beta^n + 1}. \quad (7.80)$$

When considering the P2 case, there will be some additional terms in the coefficient of the penalty term. i.e.

$$E_{n(N+1)} = 2E_{n(N)} - E_{n(N-1)} - \frac{1 - \kappa}{1 + \kappa^2} \frac{\tau P}{\beta^n + 1} \quad (7.81)$$

$$Z_{n(N+1)} = 2Z_{n(N)} - Z_{n(N-1)} - \frac{1 + \kappa}{1 + \kappa^2} \frac{\tau P}{\beta^n + 1} \quad (7.82)$$

and similar for Q2. The calculation for the boundary at $j = 0$ works the same giving, for example

$$E_{n(-1)} = 2E_{n(0)} - E_{n(1)} - \frac{1 - \kappa}{1 + \kappa^2} \frac{\tau P}{\beta - 1} \quad (7.83)$$

$$Z_{n(-1)} = 2Z_{n(0)} - Z_{n(1)} + \frac{1 + \kappa}{1 + \kappa^2} \frac{\tau P}{\beta - 1}, \quad (7.84)$$

for P2 and so on for the other prescriptions.

Stability of the boundary conditions can be shown by using the ‘top hat’ boundary data that was used for the KWB system whilst prescribing zero initial data. In these tests the boundary data is set to 1 until $t = 0.5$. Here we show the results for P2 and Q2 in figures 7.10 and 7.11, very similar to the results from KWB in figure 6.7. Again, we cannot consider the relative energy $E(t)/E(0)$ because the energy at $t = 0$ is zero.

Moving on to looking at convergence, we begin by considering the case with $\beta^n = 0$ in 1D. Here we have second order convergence for all four boundary types and

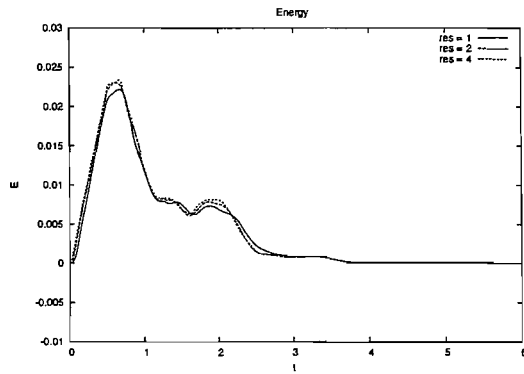


Figure 7.10: Stability of P2 boundary conditions. Top hat boundary data. 1D test.

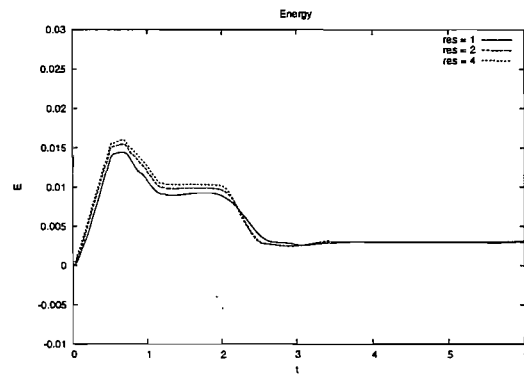


Figure 7.11: Stability of Q2 boundary conditions. Top hat boundary data. 1D test.

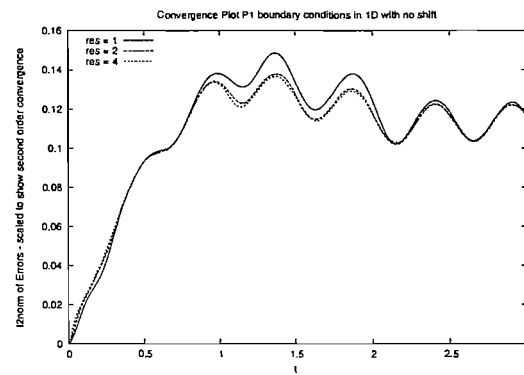


Figure 7.12: Convergence of P1 boundary conditions in 1D with no shift.

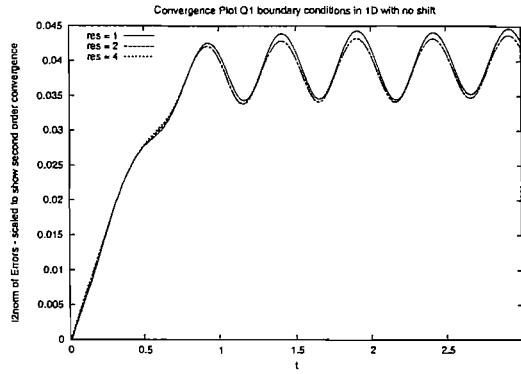


Figure 7.13: Convergence of Q1 boundary conditions in 1D with no shift.

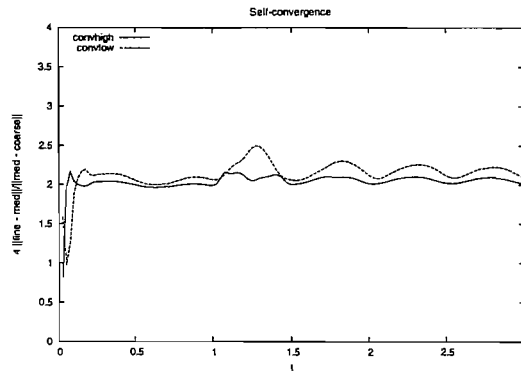


Figure 7.14: Self-convergence of P1 boundary conditions in 1D with no shift and exponentially decaying free boundary data.

non-zero values of the coupling constants. P1 and Q1 are shown here as examples in figures 7.12 and 7.13. To check that the boundary conditions are still second order convergent for arbitrary free boundary data, a sensible choice is to set the free data to zero. However, this would not then be consistent with the initial data at $t = 0$, so the exact free data was multiplied by an exponentially decaying factor to force the free data to zero

$$f_n = e^{-t}u(t). \quad (7.85)$$

This gave second order self-convergence, shown in figures 7.14 and 7.15. Despite the features, as long as the convergence is closer to 2 at the higher solution, we are satisfied with the convergence.

The next stage is to introduce a shift and again we get second order convergence for 1D and the extension to 2D. The errors are larger in 2D than in 1D but the important thing is that they are still convergent. Note that the lowest resolution

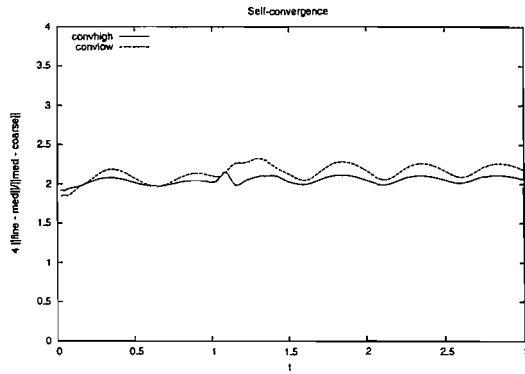


Figure 7.15: Self-convergence of Q1 boundary conditions in 1D with no shift and exponentially decaying free boundary data.

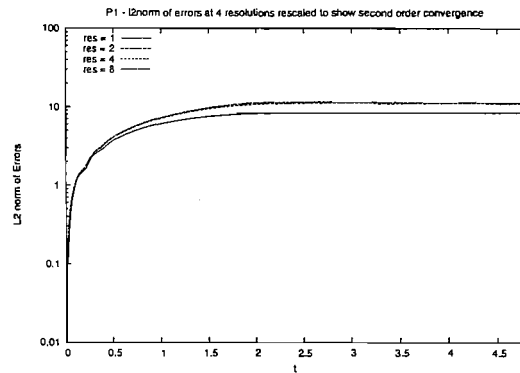


Figure 7.16: P1 boundary conditions with exact free boundary data and no shift. Rescaled l_2 norms of the errors at four different resolutions to show second order convergence.

is not coincident with the other curves. However, the higher resolution all do match and so we have convergence. With exponentially decaying free boundary data we again get second order self-convergence (figure 7.18). The same tests were performed with Q1/P2/Q2 boundary conditions and these prescriptions were also found to be second order convergent with arbitrary shift terms (figures 7.19 - 7.21).

Constraint satisfying free data X was then introduced as described above. We therefore need evolution of the auxiliary variable X on the boundary. Note that for the P-type boundary conditions X is used as the free data whereas for Q-type conditions the evolution equation of X is used as the free data. We have also made the adjustment to the specification of the free data to ensure consistency with the initial data, in a similar form to the exponentially decaying free data

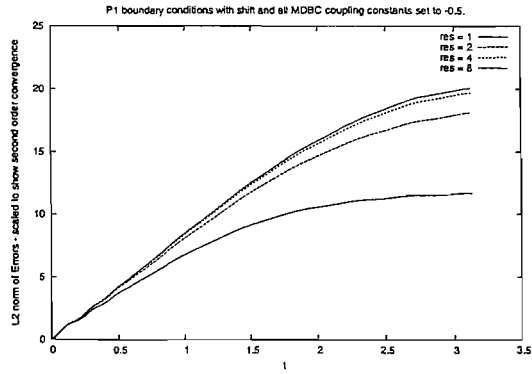


Figure 7.17: Convergence of P1 boundary conditions in 2D case with shift. All MDBC coupling constants set to -0.5.

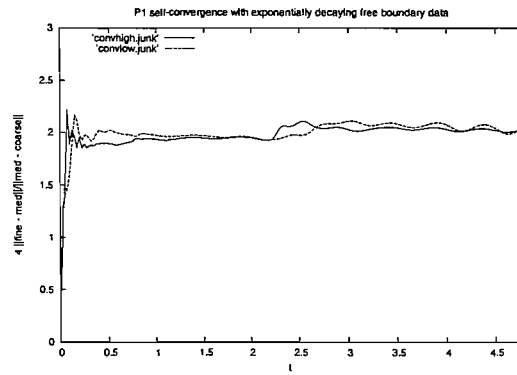


Figure 7.18: P1 boundary conditions with exponentially decaying initial data. Self-convergence using solutions at four different resolutions.

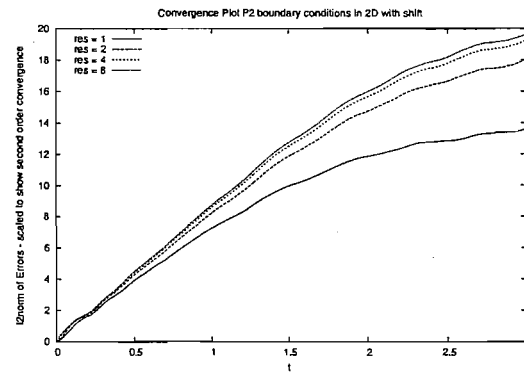


Figure 7.19: Convergence of P2 boundary conditions in 2D case with shift. All MDBC coupling constants set to -0.5.

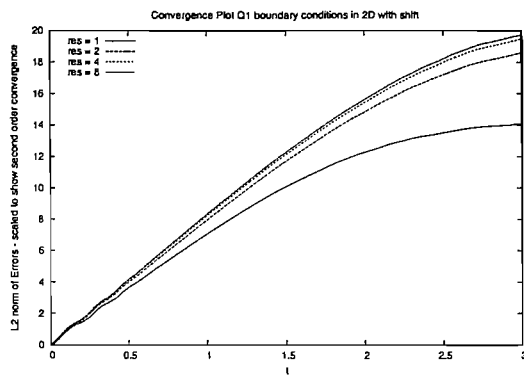


Figure 7.20: Convergence of Q1 boundary conditions in 2D case with shift. All MDBC coupling constants set to -0.5 .

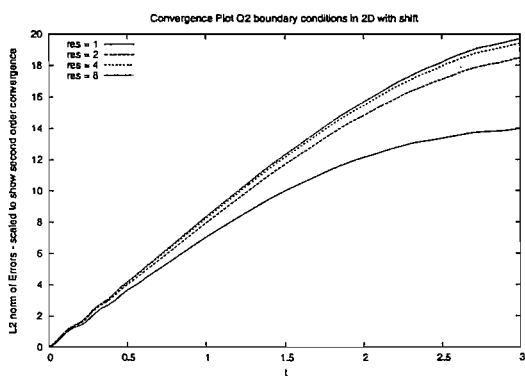


Figure 7.21: Convergence of Q2 boundary conditions in 2D case with shift. All MDBC coupling constants set to -0.5 .

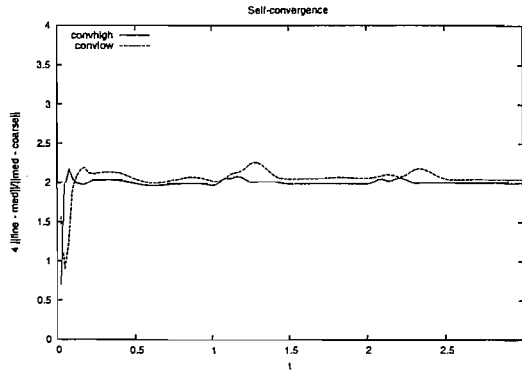


Figure 7.22: Self-convergence of constraint preserving P1 boundary conditions in 1D with no shift.

that was used to test convergence with zero free data. The form of the free data was set to be

$$e^{-t}u(t) + (1 - e^{-t})X, \quad (7.86)$$

where $u(t)$ is equal to the exact data at the boundary (but need only be anything consistent with the initial data) and X is the constraint satisfying free data. The evolution of X is calculated in the same way as for KWB, however note the difference in the definition of C_{\pm}

$$C_{\pm} = Z_{,n} \pm E_{i,i} = U_{\pm,n} \pm E_{B,B}, \quad (7.87)$$

which gives the resulting evolution for X

$$\dot{X} = \beta^A X_{,A} + (-\beta^n E_{B,B} - A_{n,BB} + A_{B,nB}) (1 + \kappa). \quad (7.88)$$

Again, we begin in 1D with no shift. We show self-convergence for the P1 and Q2 prescriptions in figures 7.22 and 7.23. There are features at about one and two crossing times showing that there are still problems with the errors introduced at $t = 0$ hitting the boundaries, however these features decrease in amplitude with increased resolution. Adding in the shift in 1D, we show in figures 7.24 and 7.25 second order convergence, however note the initial feature in figure 7.25. Convergence drops due to high frequency noise introduced from the boundary. When this noise has left the grid, second order convergence is regained. Dissipation does not fix this situation, however the problem seems to be caused at the boundary at initial time so equation (7.86) may not have solved the consistency issue at this location. Observing the time evolution pointwise self-convergence seems to show second order convergence of the solution overlaid with noise.

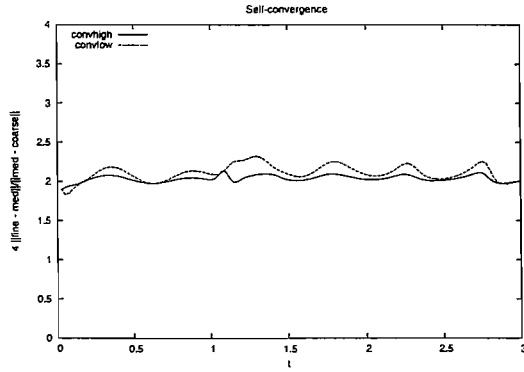


Figure 7.23: Self-convergence of constraint preserving Q2 boundary conditions in 1D with no shift.

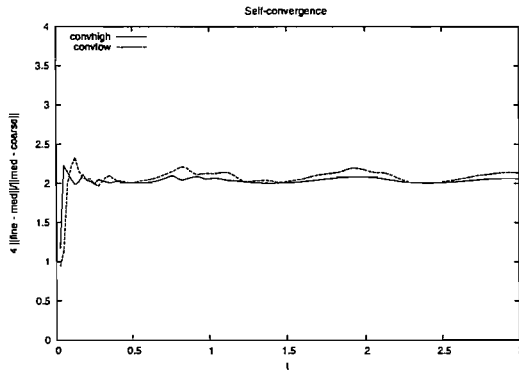


Figure 7.24: Self-convergence of constraint preserving P1 boundary conditions in 1D case with shift.

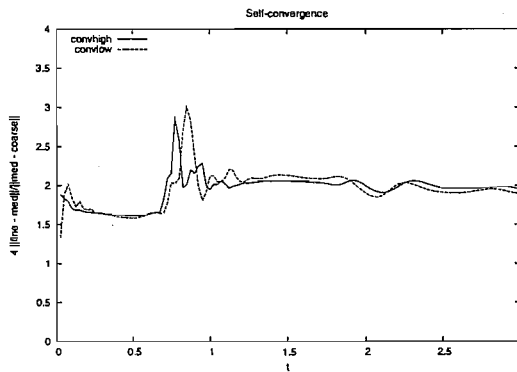


Figure 7.25: Self-convergence of constraint preserving Q1 boundary conditions in 1D case with shift.

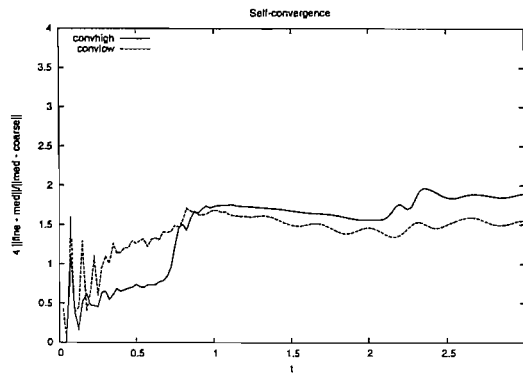


Figure 7.26: Self-convergence of constraint preserving P1 boundary conditions in 2D with shift.

Self-convergence of constraint preserving P1 and Q1 boundary conditions in 2D are shown in figures 7.26 and 7.28. With P1, second order convergence is not clear (figure 7.26) as there is a drop in convergence at early times, but this seems to be due to noise from initial time that takes two crossing times to leave the grid. Considering the evolution of the pointwise convergence, we do seem to have second order convergence, but it is clear we get unwanted noise early on. This may mean that the P-type boundary condition works less well with shift. Although it seems to work in 1D, this is not a rigorous test as the evolution of X is constructed by transverse derivatives, which are all zero in the 1D case. The constraint energy decreases at a faster rate with increase of resolution in figure 7.27 but it is still undesirably large, so it seems that the prescription is not controlling the constraint energy well. The Q-type boundary in figure 7.28 performs much better; there is clear second order self-convergence, with good control of the constraint energy in figure 7.29, tending to the limit of conserved constraint energy as resolution increases. Notice that the convergence here is clearer than in the 1D cases because we have much smaller constraint violations in the initial data in this case.

In conclusion it seems clear that the constraint preserving Q-type boundary is preferable to the P-type boundary. When carrying out 2D tests, constraint preserving P-type boundaries do not perform particularly well, both in terms of convergence and in terms of the control of the constraint energy. Q-type boundaries perform much better in both these respects.

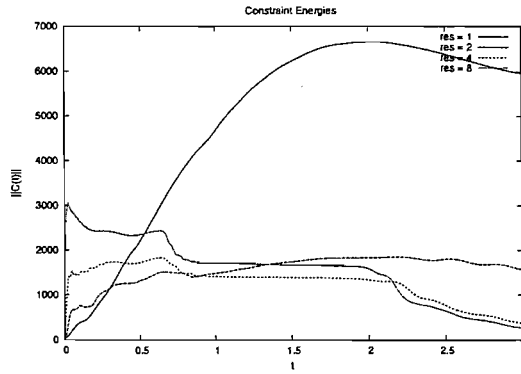


Figure 7.27: Self-convergence of constraint preserving P1 boundary conditions in 2D with shift.

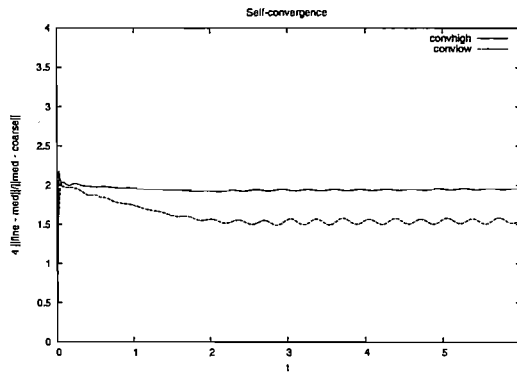


Figure 7.28: Constraint energies for constraint preserving Q1 boundary conditions in 2D with shift.

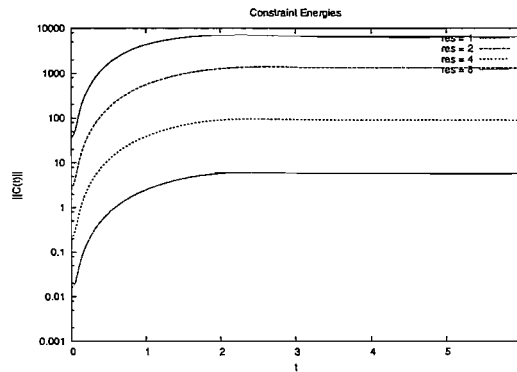


Figure 7.29: Constraint energies for constraint preserving Q1 boundary conditions in 2D with shift.

Chapter 8

Conclusions

We have prescribed second order accurate maximally dissipative boundary conditions and constraint preserving boundary conditions for the Z1 system and the KWB system, the electromagnetic analogues to the Z4 and NOR systems used in numerical relativity. To construct these boundary conditions, we have broken down the formulations into systems of equation that look like the first order and second order in space wave equations, so that boundary conditions for the wave equations can be combined to give general prescriptions for Z1 and KWB. We have also used the energy method for KWB with the boundaries prescribed; by finding a bounded, positive definite system energy, we prove stability and hence convergence. An attempt was made to carry out a similar calculation when a shift is included, however this was impossible using a technique that was valid for the wave equation. It is important to note that Z1 requires artificial dissipation to avoid an instability even in the case with periodic boundaries. It has been shown in [6] that the same instability occurs in the Z4 system, so this is not a peculiarity of the electromagnetic analogue.

The boundaries for the first order wave equation involve using a combination of first order accurate terms and penalty terms, which incorporate MDBC to drive the solution back to the surface of bounded energy. We have four separate forms of this boundary condition - P1/P2/Q1/Q2. The P-type boundary conditions make use of MDBC in the penalty term whilst Q-type conditions use the time derivative of MDBC. 1-type conditions only apply the penalty term to the information coming into the domain, whilst 2-type apply penalty terms to the information going out and that coming in to enforce that the energy of the system is explicitly bounded. All four prescriptions worked well for specific values of the parame-

ter multiplying the penalty terms, however the 2-type boundary conditions are conceptually preferable as the inherent bounding of the energy is an attractive property.

The boundaries for the second order wave equation use the MDBC directly to give a second order accurate approximation of a derivative on the boundary.

Combining these two prescriptions gives the required number of boundary conditions for both the Z1 and the KWB systems. KWB only requires the second order wave equation method and the resulting solution is second order convergent for all values of the maximally dissipative coupling constants, which couple the incoming and outgoing modes, however the Courant factor needs to be reduced as the coupling constants are increased. We also have second order convergence when the shift is introduced, with the specification of data at the boundary to the variable Γ when this variable is incoming and the use of third order extrapolation, (setting the third derivative of the variable in question to zero at the boundary) for the remaining variables.

For Z1, all four prescriptions P1/P2/Q1/Q2 seem to perform equally well, giving second order convergence when there is no shift. Incorporating the shift requires rewriting the first order wave equation boundary condition, with the penalty term requiring additional factors involving the shift. Not all variables can be treated by these boundary conditions so for variables that aren't controlled, third order extrapolation was used. Once again, all of the schemes tested were second order convergent with the exact free boundary data and second order self-convergent with arbitrary free boundary data.

Considering constraint preserving boundary conditions, we introduced an auxiliary variable at the boundary that controls the energy of the constraints and evolved this auxiliary variable, using it as 'free' boundary data in the MDBC described above. Unfortunately, the energy method cannot be used rigorously in this case because the evolution of the 'free' data is now coupled to the solution in the domain. Constraint preserving boundary conditions are second order convergent for KWB, however the situation with Z1 is not so clear. There is a clear distinction when performing 2D tests between the P-type and Q-type boundary conditions. Q-type conditions perform well in this situation in terms of self-convergence and the control of the constraint energy and are clearly preferable to P-type conditions, which are not clearly second order self-convergent and do not damp the constraint energy as strongly.

The one aspect that was not studied here was the introduction of the constraint damping parameter in the Z1 system. The introduction of this term would be interesting in that it would work in combination with CPBC to ensure no constraint violation in the grid. We can see that the CPBC for Z1 work much better when constraint violations are small, i.e. they prevent constraint violations from being injected into the grid but react less well to large constraint violations already present in the grid. Hence the damping parameter would assist by preventing constraint violations already present or appearing in the interior whilst CPBC would stop injection of violations at the boundary.

In summary, the prescription of MDBC and CPBC for the KWB system and MDBC and the Q-type CPBC for the Z1 system give second order convergence and so have been proved to be effective boundary conditions in these simple cases. These methods should be useful in NOR and Z4, however the limitation of these results should be stressed. The fact that these boundary conditions work in these simple linear cases is not a guarantee that they will work in the full non-linear GR codes but well-posedness of a linearised system is a necessary condition for well-posedness of the corresponding non-linear system so it was important to confirm results in this linear situation.

Appendix A

Derivations

A.1 Definitions of the extrinsic curvature

Here again are the four definition of K_{ab} :

$$K_{ab} = -\frac{1}{2} \perp \mathcal{L}_n g_{ab} \quad (\text{A.1})$$

$$K_{ab} = \perp \nabla_{(a} n_{b)} \quad (\text{A.2})$$

$$K_{ab} = -\frac{1}{2} \mathcal{L}_n \gamma_{ab} \quad (\text{A.3})$$

$$K_{ab} = -\nabla_a n_b - n_a a_b, \quad \text{where } a_b = n^c \nabla_c n_b \quad (\text{A.4})$$

and here are the proofs. (A.1) \Leftrightarrow (A.2)

$$\begin{aligned} -\frac{1}{2} \perp \mathcal{L}_n g_{ab} &= -\frac{1}{2} \perp (n^c \nabla_c g_{ab} + g_{cb} \nabla_a n^c + g_{ac} \nabla_b n^c) \\ &= -\frac{1}{2} \perp (\nabla_a n_b + \nabla_b n_a) \\ &= -\perp \nabla_{(a} n_{b)}, \end{aligned} \quad (\text{A.5})$$

where the first equality is the expansion of the Lie derivative and the second comes from $\nabla_a g_{bc} = 0$, allowing the metric to be taken in and out of the derivative using the Leibniz rule. It is useful to note that

$$\begin{aligned} 0 = \nabla_a n^b n_b &= n^b \nabla_a n_b + n_b \nabla_a n^b \\ &= 2n^b \nabla_a n_b, \end{aligned} \quad (\text{A.6})$$

giving

$$n^b \nabla_a n_b = 0. \quad (\text{A.7})$$

(A.3) \Leftrightarrow (A.1)

$$\begin{aligned}
-\frac{1}{2}\mathcal{L}_n\gamma_{ab} &= -\frac{1}{2}\perp\mathcal{L}_n\gamma_{ab} \\
&= -\frac{1}{2}\perp\mathcal{L}_n(g_{ab} + n_a n_b) \\
&= -\frac{1}{2}\perp(\mathcal{L}_n g_{ab} + n_a \mathcal{L}_n n_b + n_b \mathcal{L}_n n_a) \\
&= -\frac{1}{2}\perp\mathcal{L}_n g_{ab},
\end{aligned} \tag{A.8}$$

as $\mathcal{L}_n n_a = 0$ and $\mathcal{L}_n \perp_a^c = 0$.

It is also useful to note that although most references define K_{ab} in a symmetric way, this is by no means necessary as it is naturally symmetric. This can be seen by taking (A.2) without the symmetrizing condition and using the definition of $n_a = \alpha \nabla_a t$:

$$\begin{aligned}
-\perp\nabla_a n_b &= \perp\nabla_a(\alpha\nabla_b t) \\
&= \perp\nabla_b t \nabla_a \alpha + \perp\alpha\nabla_a \nabla_b t \\
&= \perp\alpha\nabla_b t \nabla_a \ln \alpha + \alpha\perp\nabla_a \nabla_b t \\
&= \perp n_b \nabla_a \ln \alpha + \alpha\perp\nabla_a \nabla_b t \\
&= \alpha\perp\nabla_a \nabla_b t,
\end{aligned} \tag{A.9}$$

which is symmetric in a and b. The first term of the fourth equality disappears because it involves the projection of n_b , which is zero. (A.2) \Leftrightarrow (A.4)

$$\begin{aligned}
-\perp\nabla_{(a} n_{b)} &= -\perp\nabla_a n_b \\
&= -\nabla_a n_b - n^c n_a \nabla_c n_b \\
&= -\nabla_a n_b - n_a a_b,
\end{aligned} \tag{A.10}$$

using the definition of a_b from (A.4).

A.2 The Gauss equation

Before beginning the derivation it will be useful to show the following result:

$$\begin{aligned}
\perp_a^b \perp_c^d \nabla_b \perp_d^e &= \perp_a^b \perp_c^d \nabla_b (\delta_d^e + n_d n^e) \\
&= n^e \perp_a^b \perp_c^d \nabla_b n_d \\
&= -n^e K_{ac},
\end{aligned} \tag{A.11}$$

where we have simply taken the definition of the projector and then used the Leibniz rule, remembering that $\nabla_a \delta_c^b = 0$ and $n_a \perp_b^a = 0$. The definition for K_{ab} (A.2) is then used to give the result.

Now, taking the commutator of the 3-D covariant derivative, we can derive the Gauss equation, which shows how the projection of the 4-D Riemann tensor splits into the 3-D Riemann tensor and extrinsic curvature terms. We begin by expanding $D_a D_b \omega_c$:

$$\begin{aligned}
D_a D_b \omega_c &= D_a (\perp_b^d \perp_c^e \nabla_d \omega_e) \\
&= \perp_a^f \perp_b^g \perp_c^k \nabla_f (\perp_g^d \perp_k^e \nabla_d \omega_e) \\
&= \perp_a^f \perp_b^d \perp_c^e \nabla_f \nabla_d \omega_e \\
&\quad + \perp_a^f \perp_b^d \perp_c^k \nabla_d \omega_e \nabla_f \perp_k^e + \perp_a^f \perp_c^e \perp_b^g \nabla_d \omega_e \nabla_f \perp_g^d \\
&= \perp_a^f \perp_b^d \perp_c^e \nabla_f \nabla_d \omega_e - \perp_b^d \nabla_d \omega_e n^e K_{ac} - \perp_c^e \nabla_d \omega_e n^d K_{ab}, \quad (\text{A.12})
\end{aligned}$$

where we have used (A.11) twice. When antisymmetrised the last term will disappear as K_{ab} is symmetric. It should also be noted that

$$\begin{aligned}
\perp_b^d n^e \nabla_d \omega_e &= \perp_b^d \nabla_d (n^e \omega_e) - \perp_b^d \omega_e \nabla_d n^e \\
&= \omega_e K_b^e. \quad (\text{A.13})
\end{aligned}$$

So, using the definitions

$${}^{(4)}R^d{}_{cba} \omega_d = \nabla_a \nabla_b \omega_c - \nabla_b \nabla_a \omega_c \quad (\text{A.14})$$

$${}^{(3)}R^d{}_{cba} \omega_d = D_a D_b \omega_c - D_b D_a \omega_c, \quad (\text{A.15})$$

we can see that:

$$\begin{aligned}
{}^{(3)}R^d{}_{cba} \omega_d &= D_a D_b \omega_c - D_b D_a \omega_c \\
&= \perp_a^f \perp_b^d \perp_c^e \nabla_f \nabla_d \omega_e - \perp_b^f \perp_b^d \perp_c^e \nabla_f \nabla_d \omega_e \\
&\quad - \perp_b^d \nabla_d \omega_e n^e K_{ac} + \perp_a^d \nabla_d \omega_e n^e K_{bc} \\
&= \perp_a^f \perp_b^d \perp_c^e (\nabla_f \nabla_d \omega_e - \nabla_d \nabla_f \omega_e) - K_{ac} \omega_e K_b^e + K_{bc} \omega_e K_a^e \\
&= \perp_a^f \perp_b^d \perp_c^e R^g{}_{edf} \omega_g - K_{ac} \omega_e K_b^e + K_{bc} \omega_e K_a^e. \quad (\text{A.16})
\end{aligned}$$

As this is true for all ω_e we can write

$${}^{(3)}R_{abcd} = \perp {}^{(4)}R_{abcd} + K_{ad} K_{bc} - K_{ac} K_{bd}, \quad (\text{A.17})$$

where we have lowered indices and used Riemann symmetries. This is the Gauss equation.

A.3 The Codazzi equation

$$\begin{aligned}
D_b K_{ac} &= \perp_b^f \perp_a^e \perp_c^g \nabla_f K_{eg} \\
&= - \perp_b^f \perp_a^e \perp_c^g \nabla_f (\perp_e^h \perp_g^k \nabla_h n_k) \\
&= - \perp_b^f \perp_a^h \perp_c^k \nabla_f \nabla_h n_k \\
&\quad - \perp_b^f \perp_a^e \perp_c^k \nabla_h n_k \nabla_f \perp_e^h - \perp_b^f \perp_a^h \perp_c^g \nabla_h n_k \nabla_f \perp_g^k \\
&= \perp_b^f \perp_a^h \perp_c^k \nabla_f \nabla_h n_k - n^h K_{ba} \perp_c^k \nabla_h n_k \\
&\quad - \perp_b^f \perp_a^h \perp_c^g \nabla_h n_k \nabla_f (\delta_g^k + n^k n_g).
\end{aligned} \tag{A.18}$$

The second term disappears when we antisymmetrize on a and b . The last term can be eliminated because the covariant derivative of δ is zero as are $\nabla_h n^k n_k$ and $\perp_b^a n_a$ leaving

$$\begin{aligned}
D_b K_{bc} - D_a K_{ac} &= - \perp_b^f \perp_a^h \perp_c^k \nabla_f \nabla_h n_k + \perp_a^f \perp_b^h \perp_c^k \nabla_f \nabla_h n_k \\
&= - \perp_b^f \perp_a^h \perp_c^k R^d{}_{khf} n_d \\
&= - \perp R_{dcab} n^d \\
&= \perp R_{abcn}.
\end{aligned} \tag{A.19}$$

This is the Codazzi equation.

A.4 The Hamiltonian constraint

Taking the Gauss equation

$${}^{(3)}R_{abcd} = \perp^{(4)} R_{abcd} + K_{ad} K_{bc} - K_{ac} K_{bd}, \tag{A.20}$$

we can contract with the spatial metric twice to give:

$$\begin{aligned}
R &= \gamma^{ac} \gamma^{bd} \perp_a^e \perp_b^f \perp_c^g \perp_d^h R_{efgh} + K_{ad} K^{da} - K^2 \\
\gamma^{eg} \gamma^{fh} R_{efgh} &= R + K^2 - K_{ab} K^{ab},
\end{aligned} \tag{A.21}$$

where we have used the definition $K \equiv \gamma^{ab} K_{ab}$ and the fact that K_{ab} is symmetric.

Now,

$$\begin{aligned}
\gamma^{eg} \gamma^{fh} R_{efgh} &= \gamma^{eg} R_{eg} + \gamma^{eg} n^f n^h R_{efgh} \\
&= R + n^e n^g R_{eg} + n^f n^h R_{fh} + n^e n^f n^g n^h R_{efgh}
\end{aligned}$$

$$\begin{aligned}
&= -n_a n^a R + 2n^a n^b R_{ab} \\
&= 2(n^a n^b R_{ab} - \frac{1}{2} n^a n^b g_{ab} R) \\
&= 2n^a n^b G_{ab} \\
&= 2G_{nn},
\end{aligned} \tag{A.22}$$

where the first two equalities use the identity $\gamma^{ab} = g^{ab} + n^a n^b$ and the third is a rearrangement of dummy indices. Hence

$$2G_{nn} = R + K^2 - K_{ab} K^{ab} = 2\kappa\rho, \tag{A.23}$$

where $\rho \equiv T_{nn}$. This is the scalar or Hamiltonian constraint.

A.5 The momentum constraint

We now contract the Codazzi equation once with the spatial metric.

$$\begin{aligned}
\gamma^{ac} \perp R_{abcn} &= \gamma^{ac} (D_b K_{ac} - D_a K_{bc}) \\
\gamma^{ac} \perp_a \perp_b^f \perp_c^g R_{efgn} &= D_b K_a^a - D_a K_b^a \\
\gamma^{eg} \perp_b^f R_{efgn} &= D_b K - D_a K_b^a.
\end{aligned} \tag{A.24}$$

Now

$$\begin{aligned}
\gamma^{eg} \perp_b^f R_{efgn} &= \perp_b^f (g^{eg} + n^e n^g) R_{efgn} \\
&= \perp_b^f R_{fn} - \perp_b^f n^e n^g R_{efgn} \\
&= \perp_b^f R_{fn},
\end{aligned} \tag{A.25}$$

as the second term disappears like before because $n^g n^h R_{efgh} = -n^h n^g R_{efhg} = -n^g n^h R_{efgh}$. We have

$$\begin{aligned}
\perp_b^f G_{fn} &= \perp_b^f R_{fn} - \frac{1}{2} \perp_b^f g_{fn} R \\
&= \perp_b^f R_{fn} - \frac{1}{2} \perp_b^f n_f R \\
&= \perp_b^f R_{fn}.
\end{aligned} \tag{A.26}$$

Hence, (A.24) can be written as

$$\perp_b^f G_{fn} = D_b K - D_a K_b^a. \tag{A.27}$$

And finally, raising indices with γ^{ab} , we obtain,

$$\begin{aligned}
\gamma^{ab} \perp_b^f G_{fn} &= \gamma^{ab}(D_b K - D_c K_b^c) \\
\gamma^{af} G_{fn} &= \gamma^{ab} D_b K - D_c K^{ac} \\
\perp_f^a G_n^f &= \gamma^{ab} D_b K - D_b K^{ab} \\
\perp G^{an} &= D_b(K^{ab} - \gamma^{ab} K) = j^a,
\end{aligned} \tag{A.28}$$

where we have used the definitions $\perp G^{an} \equiv -\perp G_n^a$ and $j^a \equiv \perp T^{an}$.

A.6 The evolution equation of the extrinsic curvature

Before calculating the Lie derivative of the curvature with respect to t^a , we need a couple more useful results. Remembering that the acceleration of the observers moving with the slices can be defined as

$$a_b \equiv n^c \nabla_c n_b, \tag{A.29}$$

we can derive $a_b = D_b \ln \alpha$

$$\begin{aligned}
D_b \ln \alpha &= \perp \nabla_b \ln \alpha \\
&= \nabla_b \ln \alpha + n^a n_b \nabla_a \ln \alpha \\
&= \alpha^{-1} \nabla_b \alpha + \alpha^{-1} n^a n_b \nabla_a \alpha \\
&= -\alpha^{-1} n^a n_a \nabla_b \alpha + \alpha^{-1} n^a n_b \nabla_a \alpha \\
&= n^a (\nabla_b t \nabla_a \alpha - \nabla_a t \nabla_b \alpha) \\
&= n^a (\nabla_a (\alpha \nabla_b t) - \alpha \nabla_a \nabla_b t - \nabla_b (\alpha \nabla_a t) + \alpha \nabla_b \nabla_a t) \\
&= n^a (\nabla_a n_b - \nabla_b n_a) \\
&= n^a \nabla_a n_b \\
&= a_b,
\end{aligned} \tag{A.30}$$

where we have used $n^a n_a = -1$, the Leibniz rule and (A.6). The final and important relation is the equation of motion of the spatial metric. Here, we use $t^a = \alpha n^a + \beta^a$.

$$\begin{aligned}
\mathcal{L}_t \gamma_{ab} &= t^c \nabla_c \gamma_{ab} + \gamma_{cb} \nabla_a t^c + \gamma_{ac} \nabla_b t^c \\
&= (\alpha n^a + \beta^a) \nabla_c \gamma_{ab} + \gamma_{cb} \nabla_a (\alpha n^c + \beta^c) + \gamma_{ac} \nabla_b (\alpha n^c + \beta^c)
\end{aligned}$$

$$\begin{aligned}
&= \alpha n^a \nabla_c \gamma_{ab} + \beta^a \nabla_c \gamma_{ab} + \alpha \gamma_{cb} \nabla_a n^c + n^c \gamma_{cb} \nabla_a \alpha \\
&\quad + \gamma_{cb} \nabla_a \beta^c + \alpha \gamma_{ac} \nabla_b n^c + n^c \gamma_{ac} \nabla_b \alpha + \gamma_{ac} \nabla_b \beta^c \\
&= \alpha \mathcal{L}_n \gamma_{ab} + \mathcal{L}_\beta \gamma_{ab} + n^c \gamma_{cb} \nabla_a \alpha + n^c \gamma_{ac} \nabla_b \alpha \\
&= -2\alpha K_{ab} + \mathcal{L}_\beta \gamma_{ab},
\end{aligned} \tag{A.31}$$

using relations (A.3) and (4.2).

So now, without using the constraints, we can derive the formula for the Lie derivative of the extrinsic curvature. First, as $\mathcal{L}_{p+q} = \mathcal{L}_p + \mathcal{L}_q$, we know that

$$\mathcal{L}_t = \mathcal{L}_N + \mathcal{L}_\beta, \tag{A.32}$$

so using (A.31) and (A.32) gives

$$L_N \gamma_{ab} = -2\alpha K_{ab}. \tag{A.33}$$

Now, we have

$$\begin{aligned}
\mathcal{L}_N(\gamma_{ab}) &= \mathcal{L}_N(\gamma_a^c \gamma_{cb}) \\
&= \gamma_a^c \mathcal{L}_N \gamma_{cb} + \gamma_{cb} \mathcal{L}_N \gamma_a^c,
\end{aligned} \tag{A.34}$$

so that

$$\begin{aligned}
-2\alpha K_{ab} &= \gamma_a^c L_N \gamma_{cb} + \gamma_{cb} L_N \gamma_a^c \\
&= -2\alpha \gamma_a^c K_{cb} + \gamma_{cb} \mathcal{L}_N \gamma_a^c,
\end{aligned} \tag{A.35}$$

which straight away gives

$$\mathcal{L}_N \gamma_a^c = 0. \tag{A.36}$$

This result is used in the following derivation of $\mathcal{L}_N K_{ab}$.

$$\begin{aligned}
\mathcal{L}_N K_{ab} &= \mathcal{L}_N(\perp \nabla_a n_b) \\
&= \mathcal{L}_N(\perp_a^c \perp_b^d \nabla_c n_d) \\
&= \perp_a^c \perp_b^d \mathcal{L}_N(\nabla_c n_d) \\
&= \perp_a^c \perp_b^d (\alpha n^e \nabla_e \nabla_c n_d + \nabla_e n_d \nabla_c (\alpha n^e) + \nabla_c n_e \nabla_d (\alpha n^e)) \\
&= \perp_a^c \perp_b^d \left(\alpha n^e \nabla_e \nabla_c n_d - \alpha n^e \nabla_c \nabla_e n_d \right. \\
&\quad \left. + \nabla_c (\alpha n^e \nabla_e n^d) + \nabla_c n_e \nabla_d (\alpha n^e) \right) \\
&= \alpha n^e \perp_a^c \perp_b^d R_{ecd}{}^f n^f + D_a(\alpha a_d) + \perp_a^c \nabla_c n_e \perp_b^d \nabla_d (\alpha n^e) \\
&= \alpha \perp R_{anbn} + D_a(\alpha D_b \ln \alpha) + \perp_a^c \nabla_c n_e \alpha \perp_b^d \nabla_d n^e \\
&= -\alpha \perp R_{anbn} + D_a D_b \alpha + \alpha K_{ac} K_b^c.
\end{aligned} \tag{A.37}$$

The only subtleties are the use of equation (A.36) in the third equality and the following result in the seventh.

$$\begin{aligned}\perp_a^c \perp_e^f \nabla_c n_f &= \perp_a^c \delta_e^f \nabla_c n_f + \perp_a^c n_e n^f \nabla_c n_f \\ &= \perp_a^c \nabla_c n_e.\end{aligned}\tag{A.38}$$

Some work is involved in translation into the standard form for the Lie derivative of the curvature. This begins with the 4D Ricci tensor

$$\begin{aligned}R_{ab} - \frac{1}{2}g_{ab}R &= \kappa T_{ab} \\ R - \frac{n}{2}R &= \kappa g^{ab}T_{ab} \\ R &= \kappa \frac{2}{2-n} g^{cd}T_{cd},\end{aligned}\tag{A.39}$$

where n is the dimension, in this case 4. So,

$$\begin{aligned}R_{ab} &= \kappa(T_{ab} + \frac{1}{2-n}g_{ab}g^{cd}T_{cd}) \\ &= \kappa(T_{ab} - \frac{1}{2}g_{ab}g^{cd}T_{cd}).\end{aligned}\tag{A.40}$$

If we define

$$S_{ab} \equiv \perp T_{ab},\tag{A.41}$$

then

$$\begin{aligned}S_{ab} &= \perp_a^c \perp_b^d T_{cd} \\ &= T_{ab} + n^c n_a T_{cb} + n^d n_b T_{ad} + N_a n_b n^c n^d T_{cd} \\ &= T_{ab} + \delta_b^d n_a T_{nd} + n_a n_b n^d T_{nd} + \delta_a^c n_b T_{cn} + n_a n_b n^c T_{cn} - n_a n_b T_{nn} \\ &= T_{ab} + \perp n_{(a} T_{nb)} - n_a n_b T_{nn}\end{aligned}\tag{A.42}$$

and

$$T_{ab} = S_{ab} + 2j_{(a} n_{b)} + \rho n_a n_b.\tag{A.43}$$

Now we can write

$$\begin{aligned}\mathcal{L}_t K_{ab} &= \mathcal{L}_N K_{ab} + \mathcal{L}_\beta K_{ab} \\ &= \alpha \perp R_{anbn} - \alpha K_{ac} K_b^c - D_a D_b \alpha + \mathcal{L}_\beta K_{ab} \\ &= -D_a D_b \alpha + \alpha(\perp R_{anbn} - K_{ac} K_b^c) + \mathcal{L}_\beta K_{ab}.\end{aligned}\tag{A.44}$$

So we take

$$\perp R_{anbn} = \perp_a^e \perp_b^f R_{egfh} n^g n^h$$

$$\begin{aligned}
&= \perp_a^e a \perp_b^f \gamma^{gh} R_{efgh} - \perp_a^e \perp_b^f g^{gh} R_{efgh} \\
&= \gamma^{cd} \perp_a^e \perp_b^f \perp_c^g \perp_d^h R_{efgh} - \perp R_{ef} \\
&= \gamma^{cd} (\perp R_{acbd}) - \perp R_{ef} \\
&= \gamma^{cd} ({}^{(3)}R_{acbd} + K_{ab}K_{cd} - K_{ad}K_{cb}) - \perp R_{ef} \\
&= ({}^{(3)}R_{ab} + K_{ab}K - K_{ad}K_b^d) - \perp R_{ef}
\end{aligned} \tag{A.45}$$

and

$$\begin{aligned}
-\perp R_{ef} &= -\kappa \perp (T_{ab} - \frac{1}{2}g_{ab}g^{cd}T_{cd}) \\
&= -\kappa (S_{ab} - \frac{1}{2} \perp g_{ab}(-\rho + S)) \\
&= -\kappa (S_{ab} - \frac{1}{2} \perp_a^c \perp_b^d g_{cd}(-\rho + S)) \\
&= -\kappa (S_{ab} - \frac{1}{2}\gamma_{ab}S) - \frac{1}{2}\kappa\rho\gamma_{ab}.
\end{aligned} \tag{A.46}$$

These can be put together to give

$$\begin{aligned}
\mathcal{L}_t K_{ab} &= -D_a D_b \alpha + \alpha [R_{ab} - 2K_{ac}K_b^c + K_{ab}K \\
&\quad - \kappa (S_{ab} - \frac{1}{2}\gamma_{ab}S) - \frac{1}{2}\kappa\rho\gamma_{ab}] + \mathcal{L}_\beta K_{ab},
\end{aligned} \tag{A.47}$$

the evolution equation of the extrinsic curvature.

Appendix B

Electromagnetic 3+1 Split

Here, we derive the 3+1 split of the Maxwell equations from their differential form

$$\underline{\nabla} \cdot \mathbf{B} = 0 \quad (\text{B.1})$$

$$\dot{\mathbf{B}} = -\underline{\nabla} \times \mathbf{E} \quad (\text{B.2})$$

$$\underline{\nabla} \cdot \mathbf{E} = 4\pi\rho \quad (\text{B.3})$$

$$\dot{\mathbf{E}} = \underline{\nabla} \times \mathbf{B} - 4\pi\mathbf{j}. \quad (\text{B.4})$$

To satisfy (B.1), a vector potential for \mathbf{B} can be introduced

$$\mathbf{B} = \underline{\nabla} \times \mathbf{A} \Rightarrow \underline{\nabla} \cdot \mathbf{B} = 0. \quad (\text{B.5})$$

Therefore from (B.2) and (B.5)

$$\underline{\nabla} \times \dot{\mathbf{A}} = -\underline{\nabla} \times \mathbf{E} \quad (\text{B.6})$$

and

$$\dot{\mathbf{A}} = -\mathbf{E} - \underline{\nabla}\psi, \quad (\text{B.7})$$

with ψ introduced as the electric potential. Hence, rewriting in index notation,

$$\dot{A}_i = -E_i - \partial_i\psi. \quad (\text{B.8})$$

Finally from (B.4),

$$\dot{\mathbf{E}} = \underline{\nabla} \times \underline{\nabla} \times \mathbf{A} - 4\pi\mathbf{j} \quad (\text{B.9})$$

and hence

$$\dot{E}_i = A_{j,ji} - A_{i,jj} - 4\pi j_i. \quad (\text{B.10})$$

The only equation that has not been incorporated is (B.3), which is translated into a constraint $C \equiv E_{i,i} - 4\pi\rho$. The system can be written out as

$$\dot{A}_i = -E_i - \psi_{,i} \quad (\text{B.11})$$

$$\dot{E}_i = A_{j,ji} - A_{i,jj} - 4\pi j_i \quad (\text{B.12})$$

$$0 = C \equiv E_{i,i} - 4\pi\rho. \quad (\text{B.13})$$

E_i is the electric field, A_i is the magnetic potential, ψ is the electric potential and j_i and ρ are source terms that satisfy $j^i_{,i} + \dot{\rho} = 0$.

Appendix C

Summation by Parts

With no boundary, we can take the scalar product of u_i and $D_0 v_i$ to give

$$\begin{aligned}
 \sum_{i=-\infty}^{\infty} u_i D_0 v_i &= \frac{1}{2h} \left(\sum_{i=-\infty}^{\infty} u_i v_{i+1} - \sum_{i=-\infty}^{\infty} u_i v_{i-1} \right) \\
 &= \frac{1}{2h} \left(\sum_{j=-\infty}^{\infty} u_{j-1} v_j - \sum_{j=-\infty}^{\infty} u_{j+1} v_j \right) \\
 &= - \sum_{i=-\infty}^{\infty} v_i D_0 u_i.
 \end{aligned} \tag{C.1}$$

For D_{\pm} we have

$$\sum_{i=-\infty}^{\infty} u_i D_{\pm} v_i = - \sum_{i=-\infty}^{\infty} v_i D_{\mp} u_i. \tag{C.2}$$

When we introduce a boundary at $j = 0$ there are some terms remaining at the boundary. Some useful identities are

$$h \sum_1^{\infty} v_i D_- u_i + u_0 v_1 = -h \sum_1^{\infty} u_i D_+ v_i \tag{C.3}$$

$$h \sum_1^{\infty} v_i D_- u_i + u_0 v_0 = -h \sum_0^{\infty} u_i D_+ v_i \tag{C.4}$$

$$2h \sum_1^{\infty} v_i D_0 u_i + u_0 v_1 + u_1 v_0 = -2h \sum_1^{\infty} u_i D_0 v_i \tag{C.5}$$

$$2h \sum_{-\infty}^{N-1} v_i D_0 u_i = -2h \sum_{-\infty}^{N-1} u_i D_0 v_i + u_N v_{N-1} + u_{N-1} v_N. \tag{C.6}$$

Appendix D

Scalar Product and Norm

D.1 The Cauchy-Schwarz inequality

$$(u, u)(v, v) \geq |(u, v)|^2, \quad (\text{D.1})$$

where $(u, v) = \bar{u}v$ is a scalar product with properties

$$(u, v) = \overline{(v, u)} \quad (\text{D.2})$$

$$(u + w, v) = (u, v) + (w, v) \quad (\text{D.3})$$

$$(u, v) \leq |u| \cdot |v|. \quad (\text{D.4})$$

Proof:

$$(u + \lambda v, u + \lambda v) \geq 0, \quad (\text{D.5})$$

where λ is a complex constant. So expanding gives

$$(u, u) + \bar{\lambda}(v, u) + \lambda(u, v) + \lambda\bar{\lambda}(v, v) \geq 0. \quad (\text{D.6})$$

Now, let

$$\lambda = \frac{-(v, u)}{(v, v)} \quad (\text{D.7})$$

and so

$$\bar{\lambda} = \frac{-(u, v)}{(v, v)}, \quad (\text{D.8})$$

so substituting this into (D.6) gives

$$(u, u) - \frac{(u, v)}{(v, v)}(v, u) - \frac{(v, u)}{(v, v)}(u, v) + \frac{(v, u)}{(v, v)} \frac{(u, v)}{(v, v)}(v, v) \geq 0 \quad (\text{D.9})$$

and hence cancellation and rearrangement gives

$$\begin{aligned}(u, u)(v, v) - (v, u)(u, v) &\geq 0 \\ (u, u)(v, v) &\geq |(u, v)|^2\end{aligned}\tag{D.10}$$

and equivalently

$$\|u\| \cdot \|v\| \geq |(u, v)|.\tag{D.11}$$

D.2 The triangle inequality

$$\|u + v\| \leq \|u\| + \|v\|.\tag{D.12}$$

Proof:

$$\begin{aligned}\|u + v\|^2 &= (u + v, u + v) \\ &= (u, u) + (v, v) + (v, u) + (u, v) \\ &= (u, u) + (v, v) + \overline{(u, v)} + (u, v) \\ &= (u, u) + (v, v) + 2\operatorname{Re}[(u, v)] \\ &\leq (u, u) + (v, v) + 2|(u, v)| \\ &\leq (u, u) + (v, v) + 2(u, u)(v, v) \\ &= (\|u\| + \|v\|)^2,\end{aligned}\tag{D.13}$$

where the Cauchy-Schwarz inequality from above has been used. These two results work in exactly the same way for other scalar products and norms.

D.3 The complex square

Consider

$$\begin{aligned}|\sqrt{\epsilon}Z_1 \pm \frac{1}{\sqrt{\epsilon}}Z_2|^2 &= (\sqrt{\epsilon}Z_1 + \frac{1}{\sqrt{\epsilon}}Z_2)(\sqrt{\epsilon}\bar{Z}_1 + \frac{1}{\sqrt{\epsilon}}\bar{Z}_2) \\ &= \epsilon|Z_1|^2 + \epsilon^{-1}|Z_2|^2 \pm Z_1\bar{Z}_2 \pm \bar{Z}_1Z_2 \\ &= \epsilon|Z_1|^2 + \epsilon^{-1}|Z_2|^2 \pm 2\operatorname{Re}[Z_1\bar{Z}_2],\end{aligned}\tag{D.14}$$

$$\tag{D.15}$$

so that

$$\epsilon|Z_1|^2 + \epsilon^{-1}|Z_2|^2 \pm 2\operatorname{Re}[Z_1\bar{Z}_2] \geq 0\tag{D.16}$$

and therefore

$$\epsilon|Z_1|^2 + \epsilon^{-1}|Z_2|^2 \geq 2\operatorname{Re}[Z_1\bar{Z}_2].\tag{D.17}$$

Bibliography

- [1] G. Nagy, O.E. Ortiz, O.A. Reula, Phys. Rev. D **70**, 044012 (2004).
- [2] M. Shibata, T. Nakamura, Phys. Rev. D **52**, 5428 (1995).
- [3] T.W. Baumgarte, S.L. Shapiro, Phys. Rev. D **59**, 024007 (1999)
- [4] C. Bona, T. Ledvinka, C. Palenzuela, M. Záček, Phys. Rev. D **67**, 104005 (2003).
- [5] H-O. Kreiss, H. U. Busenhardt, *Time-dependent Partial Differential Equations and Their Numerical Solution* (Birkhäuser, 2001)
- [6] G. Calabrese, I. Hinder, S Husa, *Numerical Stability for Finite Difference Approximations of Einstein's Equations* (2005) eprint gr-qc/0503056.
- [7] B. Gustafsson, H.O. Kreiss and J. Olinger, *Time Dependent Problems and Difference Methods* (Wiley, NY, 1995).
- [8] J.W. Thomas, *Numerical Partial Differential Equations - Finite Difference Methods* (Springer, NY, 1995).
- [9] J. W. York Jr., in *Sources of Gravitational Radiation*, edited by L. L. Smarr (Cambridge University Press, Cambridge, 1979), pp. 83-126
- [10] R. M. Wald, *General Relativity* (The University of Chicago Press, 1984).
- [11] L. Smarr, J.W. York, Jr., Phys. Rev. D **17**, 2529 (1978).
- [12] C. Gundlach, J. M. Martín-García, Phys. Rev. D **70**, 044032 (2004).
- [13] O. Sarbach, G. Calabrese, J. Pullin, M. Tiglio, Phys. Rev. D **66**, 064002 (2002)
- [14] C. Gundlach, G. Calabrese, I. Hinder, J. M. Martín-García, Class. Quant. Grav. **22**, 3767-3774 (2005).

- [15] C. Gundlach, J. M. Martín-García, Phys. Rev. D **70**, 044031 (2004).
- [16] <http://www.cactuscode.org/>
- [17] B. Szilagzi, J. Winicour, Phys. Rev. D **68**, 041501 (2003).
- [18] G. Calabrese, Class. Quant. Grav **21**, 4025-4040 (2004).
- [19] G. Calabrese, L. Lehner, M. Tiglio, Phys. Rev. D **65**, 104031 (2002).
- [20] L. Lehner, D. Neilsen, O. Reula, M. Tiglio, Class. Quant. Grav **21**, 5819-5848 (2004).
- [21] H. Shinkai, G. Yoneda, *Re-formulating the Einstein equations for stable numerical simulations* (2002) eprint gr-qc/0209111.
- [22] C. Bona, J. Massó, E. Siedel, J. Stela, Phys. Rev. D **56**, 3405 (1997).
- [23] P. Olsson, Math. Comput. **64**, 1035 (1995).
- [24] H-O. Kreiss, J. Lorenz, *Initial-Boundary Value Problems and the Navier-Stokes Equations* (Siam, 2004).
- [25] A. M. Knapp, E. J. Walker, T.W. Baumgarte, Phys. Rev. D **65**, 064031 (2002).