Chapter 6.
Boundary Conditions

O God! I could be bounded in a nutshell,
and count myself a king of infinite space,
were it not that I have bad dreams.
— *W. Shakespeare, Hamlet II, ii (1601)*

The difficulties caused by boundary conditions in scientific computing would be hard to overemphasize. Boundary conditions can easily make the difference between a successful and an unsuccessful computation, or between a fast and a slow one. Yet in many important cases, there is little agreement about what the proper treatment of the boundary should be.

One of the sources of difficulty is that although some numerical boundary conditions come from discretizing the boundary conditions for the continuous problem, other "artificial" or "numerical boundary conditions" do not. The reason is that the number of boundary conditions required by a finite difference formula depends on its stencil, not on the equation being modeled. Thus even a complete mathematical understanding of the initial boundary value problem to be solved—which is often lacking—is in general not enough to ensure a successful choice of numerical boundary conditions. This situation reaches an extreme in the design of what are variously known as "open", "radiation", "absorbing", "non-reflecting", or "far-field" boundary conditions, which are numerical artifacts designed to limit a computational domain in a place where the mathematical problem has no boundary at all.

Despite these remarks, perhaps the most basic and useful advice one can offer concerning numerical boundary conditions is this: before worrying about discretization, make sure to understand the mathematical problem. If the IBVP is ill-posed, no amount of numerical cleverness will lead to a successful computation. This principle may seem too obvious to deserve mention, but it is surprising how often it is forgotten.

[Only portions of this chapter have been written so far. The preceding typewritten pages from Chapter 5, however, include some of the material that belongs here.]

6.2. Scalar hyperbolic equations

[This section is not yet properly written, but some of the essential ideas are summarized below.]

z and κ. The following are standard abbreviations:

$$v_j^n = z^n \kappa^j = e^{i(\xi x + \omega t)}, \qquad z = e^{i\omega k}, \qquad \kappa = e^{i\xi h}. \tag{6.2.1}$$

Thus z is the "temporal amplification factor" and κ is the "spatial amplification factor" for a wave mode $e^{i(\xi x+\omega t)}$. We shall often write x and t, as here, even though the application may involve only their discretizations x_j and t_n.

History. The four papers listed first in the references for this chapter fit the following neat pattern. The 1970 paper by Kreiss is the classic reference on well-posedness of initial boundary value problems, and the 1986 paper by Higdon presents an interpretation of this theory in terms of dispersive wave propagation. The 1972 "GKS" paper by Gustafsson, Kreiss, and Sundström is the classic reference on stability of finite difference models of initial boundary value problems (although there are additional important references by Strang, Osher, and others), and the 1984 paper by Trefethen presents the dispersive waves interpretation for that.

Leftgoing and rightgoing waves. For any real frequency ω (i.e., $|z|=1$), a three-point finite difference formula typically admits two wave numbers ξ (i.e., κ), and often, one will have $c_g \ge 0$ and the other $c_g \le 0$. This is true, for example, for the leap frog and Crank-Nicolson models of $u_t = u_x$. We shall label these wave numbers ξ_L and ξ_R, for "leftgoing" and "rightgoing".

Interactions at boundaries and interfaces. If a plane wave hits a boundary or interface, then typically a reflected wave is generated that has the same ω (i.e., z) but different ξ (i.e., κ). The reflected value ξ must also satisfy the finite difference formula for the same ω, so for the simple formulas mentioned above, it will simply be the "other" value, e.g., ξ_R at a left-hand boundary.

Reflection coefficients. Thus at a boundary it makes sense to look for single-frequency solutions of the form

$$v_j^n = z^n(\alpha_L \kappa_L^j + \alpha_R \kappa_R^j) = e^{i\omega t}(\alpha_L e^{i\xi_L x} + \alpha_R e^{i\xi_R x}). \tag{6.2.1}$$

If there is such a solution, then it makes sense to define the **reflection coefficient** $R(\omega)$ by

$$R(\omega) = \frac{\alpha_R}{\alpha_L}. \tag{6.2.3}$$

Stable and unstable boundary conditions. Very roughly, the GKS theory asserts that a left-hand boundary condition is stable if and only if it admits no solutions (6.2.2) with $\alpha_L = 0$. The idea is that such a solution corresponds to spurious energy radiating into the domain from nowhere. Algebraically, one checks for stability by checking whether there are any modes (6.2.2) that satisfy three conditions:

(1) v_j^n satisfies the interior finite difference formula;

(2) v_j^n satisfies the discrete boundary conditions;

(3) v_j^n is a "rightgoing" mode; that is, either
(a) $|z| = |\kappa| = 1$ and $c_g \geq 0$, or
(b) $|z| \geq 1 > |\kappa|$.

Finite vs. infinite reflection coefficients. If $R(\omega) = \infty$ for some ω, the boundary condition must be unstable, because that implies $\alpha_L(\omega) = 0$ above. The converse, however, does not hold. That is, $R(\omega)$ may be finite if $\alpha_R(\omega)$ and $\alpha_L(\omega)$ happen to be zero simultaneously, and this is a situation that comes up fairly often. A boundary instability tends to be more pronounced if the associated reflection coefficient is infinite. However, a pronounced instability is sometimes less dangerous than a weak one, for it is less likely to go undetected.

The effect of dissipation. Adding dissipation, or shifting from centered to one-sided interior or boundary formulas, often makes an unstable model stable. Theorems to this effect can be found in various papers by Goldberg & Tadmor; see the references. However, dissipation is not a panacea, for if a slight amount of dissipation is added to an unstable formula, the resulting formula may be technically stable but still subject to oscillations large enough to be troublesome.

Hyperbolic problems with two boundaries. A general theorem by Kreiss shows that in the case of a finite difference model of a linear hyperbolic system of equations on an interval such as $x \in [0,1]$, the two-boundary problem is stable if and only if each of the two boundary conditions is individually stable.

Hyperbolic problems in corners. Analogously, one might expect that if a hyperbolic system of equations in two space variables x and y is modeled with stable boundary conditions for $x \geq 0$ and for $y \geq 0$, then the same problem would be stable in the quarter-domain $x \geq 0$, $y \geq 0$. However, examples by Osher and Sarason & Smoller show that this is not true in general.

(a) $v_0^{n+1} = v_1^n$ (b) $v_0^{n+1} = v_1^{n+1}$

Figure 6.2.1. Stable and unstable left-hand boundary conditions for the leap frog model of $u_t = u_x$ with $\lambda = 0.9$, $v = 0$ at the right-hand boundary, initial data exact.

EXERCISES

▷ *6.2.1. Interpretation of Figure 6.2.1.* In Figure 6.2.1*(b)*, various waves are evidently propagating back and forth between the two boundaries. In each of the time segments marked *a*, *b*, *c*, and *d*, one particular mode (6.2.1) dominates. What are these four modes? Explain your answer with reference to a sketch of the dispersion relation.

▶ *6.2.2. Experiments with Crank-Nicolson.*

Go back to your program of Exercise 3.2.1, and modify it now to implement CN_x—the Crank-Nicolson model of $u_t = u_x$. This is not a method one would use in practice, since there's no need for an implicit formula in this hyperbolic case, but there's no harm in looking at it as an example.

The computations below should be performed on the interval $[0,1]$ with $h = 0.01$ and $\lambda = 1$. Let $f(x)$ be defined by

$$f(x) = e^{-400(x-1/2)^2},$$

and let the boundary conditions at the endpoints be $v_0^{n+1} = v_{1/h}^{n+1} = 0$, except where otherwise specified.

(a) Write the down the dispersion relation for CN_x model of $u_t = u_x$, and sketch it. In the problems below, you should refer to this sketch repeatedly. Also write down the group velocity formula.

(b) Plot the computed solutions $v(x,t)$ at time $t = 0.25$ for the initial data $v(x,0) =$

(i) $f(x)$, *(ii)* $(-1)^j f(x)$, *(iii)* $\mathrm{Re}\{i^j f(x)\}$,

and explain your results. In particular, explain why much more dispersion is apparent in *(iii)* than in *(i)* or *(ii)*.

(c) Plot the computed solutions at time $t = 0.75$ for initial data $v(x,0) = f(x)$ and left-hand boundary conditions

(i) $v_0^{n+1} = v_1^{n+1}$, *(ii)* $v_0^{n+1} = v_1^n$,

(iii) $v_0^{n+1} = v_2^{n+1}$, *(iv)* $v_0^{n+1} = -v_1^{n+1} + v_2^{n+1} + v_3^{n+1}$.

To implement *(iv)*, you will have to make a small modification in your tridiagonal solver.

(d) Repeat *(c)* for the initial data $v(x,0) = g(x) = \max\{1 - 10|x - 1/2|, 0\}$.

(e) On the basis of *(c)* and *(d)*, which boundary conditions would you say appear stable? (Remember, stability is what we need for convergence, and for convergence, the error must decay to zero as $k \to 0$. If you are in doubt, try doubling or halving k to see what the effect on the computed solution is.)

(f) Prove that boundary condition *(i)* is stable or unstable (whichever is correct).

(g) Likewise *(ii)*.

(h) Likewise *(iii)*.

(i) Likewise *(iv)*.

6.4. Absorbing boundary conditions

A recurring problem in scientific computing is the design of **artificial boundaries**. How can one limit a domain numerically, to keep the scale of the computation within reasonable bounds, yet still end up with a solution that approximates the correct result for an unbounded domain?* For example, in the calculation of the transonic flow over an airfoil, what boundary conditions are appropriate at an artificial boundary downstream? In an acoustical scattering problem, what boundary conditions are appropriate at a spherical artificial boundary far away from the scattering object?

Artificial boundary conditions designed to achieve this kind of effect go by many names, such as **absorbing**, **nonreflecting**, **open**, **radiation**, **invisible** or **far-field** boundary conditions. Except in special situations, a perfect artificial boundary cannot be designed even in principle. After all, in the exact solution of the problem being modeled, interactions might occur outside the boundary which then propagate back into the computational domain at a later time. In practice, however, artificial boundaries can often do very well.

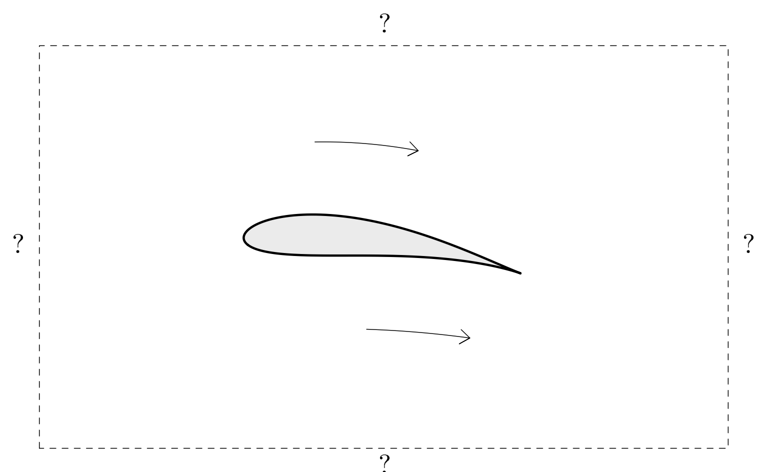


Figure 6.4.1. The problem of artificial boundaries.

There are three general methods of coping with unbounded domains in numerical simulations:

1. Stretched grids; change of variables. By a change of variables, a infinite domain can be mapped into a finite one, which can then be treated by a finite grid. Of course the equation being solved changes in the process. A closely related idea is to stay in the original physical domain, but use a stretched grid that has only finitely many grid

*Experimentalists have the same problem—how can the walls of a wind tunnel be designed to influence the flow as little as possible?

points. Methods of this kind are appealing, but for most problems they are not the best approach.

2. Sponge layers. Another idea is to surround the region of physical interest by a layer of grid points in which the same equations are solved, except with an extra dissipation term added to absorb energy and thereby prevent reflections. This "sponge layer" might have a width of, say, 5 to 50 grid points.

3. One-way equations; matched solutions. A third idea is to devise more sophisticated boundary conditions that allow propagation of energy out of the domain of interest but not into it. In some situations such a boundary condition can be obtained as a discretization of a "one-way equation" of some kind. More generally, one can think of matching the solution in the computational domain to some known outer solution that is valid near infinity, and then design boundary conditions analytically that are consistent with the latter. (See, e.g., papers by H. B. Keller and T. Hagstrom.)

Of these three methods, the first and second have a good deal in common. Both involve padding the computational domain by "wasted" points whose only function is to prevent reflections, and in both cases, the padding must be handled smoothly if the absorption is to be successful. This means that a stretched grid should stretch smoothly, and an artificial dissipation term should be turned on smoothly. Consequently the region of padding must be fairly thick, and hence is potentially expensive, especially in two or three space dimensions. On the other hand these methods are quite general.

The third idea is quite different and more problem-dependent. When appropriate one-way boundary conditions can be devised, their effect may be dramatic. As a rule of thumb, perhaps it is safe to say that effective one-way boundary conditions can usually be found if the boundary is far enough out that the physics in that vicinity is close to linear. Otherwise, some kind of a sponge layer is probably the best idea.

Of course, various combinations of these three ideas have also been considered. See, for example, S. A. Orszag and M. Israeli, *J. Comp. Phys.*, 1981.

The remainder of this section will describe a method for designing one-way boundary conditions for acoustic wave calculations which was developed by Lindman in 1975 (*J. Comp. Phys.*) and by Engquist and Majda in 1977 (*Math. Comp.*) and 1979 (*Comm. Pure & Appl. Math.*). Closely related methods were also devised by Bayliss and Turkel in 1980 (*Comm. Pure & Appl. Math.*).

For the second-order wave equation

$$u_{tt} = u_{xx} + u_{yy}, \tag{6.4.1}$$

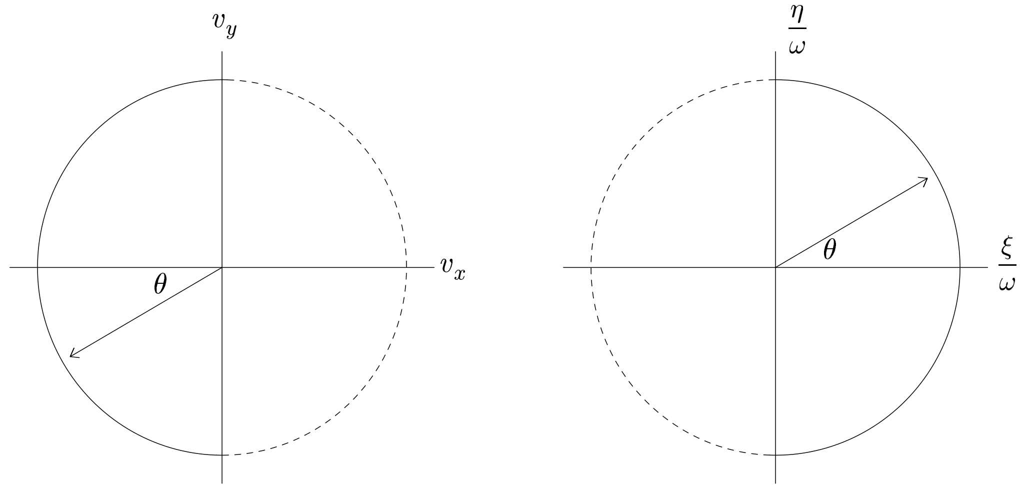
the dispersion relation for wave modes $u(x,y,t) = e^{i(\omega t + \xi x + \eta y)}$ is $\omega^2 = \xi^2 + \eta^2$, or equivalently

$$\boxed{\xi = \pm\omega\sqrt{1-s^2}, \qquad \textit{DISPERSION RELATION FOR WAVE EQUATION}} \tag{6.4.2}$$

with

$$s = \frac{\eta}{\omega} = \sin\theta \in [-1,1], \qquad \theta \in [-90°, 90°]. \tag{6.4.3}$$

This is the equation of a circle in the $\frac{\xi}{\omega} - \frac{\eta}{\omega}$ plane corresponding to plane waves propagating in all directions. The wave with wave numbers ξ, η has velocity $c = c_g = (-\frac{\xi}{\omega}, -\frac{\eta}{\omega}) = (-\cos\theta, -\sin\theta)$, where θ is the angle counterclockwise from the negative x axis. See Figure 6.4.2.



(a) space *(b)* Fourier space

Figure 6.4.2. Notation for the one-way wave equation.

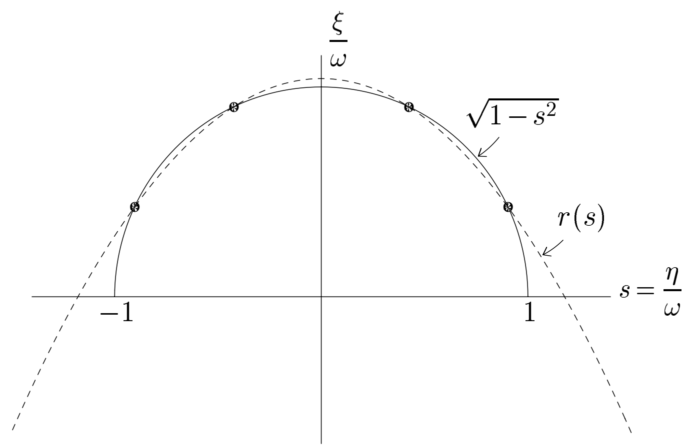


Figure 6.4.3. The approximation problem: $r(s) \approx \sqrt{1-s^2}$.

By taking the plus or minus sign in (6.4.2) only, we can restrict attention to leftgoing ($|\theta| \le 90°$) or rightgoing ($|\theta| \ge 90°$) waves, respectively. For definiteness we shall choose the former course, which is appropriate to a left-hand boundary, and write

$$\xi = +\omega\sqrt{1-s^2}. \qquad \textit{DISPERSION RELATION FOR IDEAL O.W.W.E.} \tag{6.4.4}$$

See Figure 6.4.2 again.

Because of the square root, (6.4.4) is not the dispersion relation of any partial differential equation, but of a pseudodifferential equation. The idea behind practical one-way wave equations is to replace the square root by a rational function $r(s)$ of type (m,n) for some m

and n, that is, the ratio of a polynomial p_m of degree m and a polynomial q_n of degree n,

$$r(s) = \frac{p_m(s)}{q_n(s)}.$$

Then (6.4.4) becomes

$$\boxed{\xi = \omega r(s) \qquad \textit{DISPERSION RELATION FOR APPROXIMATE O.W.W.E.}} \tag{6.4.5}$$

for the same range (6.4.4) of s and θ. See Figure 6.4.3. By clearing denominators, we can transform (6.4.5) into a polynomial of degree $\max\{m, n+1\}$ in ω, ξ, and η, and this is the dispersion relation of a true differential equation.

The standard choice of the approximation $r(s) = r_{mn}(s)$ is the **Padé approximant** to $\sqrt{1-s^2}$, which is defined as that rational function of the prescribed type whose Taylor series at $s=0$ matches the Taylor series of $\sqrt{1-s^2}$ to as high an order as possible. Assuming that m and n are even, the order will be

$$r_{mn}(s) - \sqrt{1-s^2} = O(s^{m+n+2}). \tag{6.4.6}$$

For example, the type $(0,0)$ Padé approximant to $\sqrt{1-s^2}$ is $r(s) = 1$. Taking this choice in (6.4.5) gives

$$\xi = \omega, \qquad \text{i.e.,} \qquad u_x = u_t. \tag{6.4.7}$$

This simple advection equation is thus a suitable low-order absorbing boundary condition for the wave equation at a left-hand boundary. For a numerical simulation, one would discretize it by a one-sided finite difference formula. In computations (6.4.7) is much better than a Neumann or Dirichlet boundary condition at absorbing outgoing waves.

At the next order, the type $(2,0)$ Padé approximant to $\sqrt{1-s^2}$ is $r(s) = 1 - \frac{1}{2}s^2$. Taking this choice in (6.4.5) gives

$$\xi = \omega(1 - \tfrac{1}{2}\eta^2/\omega^2),$$

that is,

$$\xi\omega = \omega^2 - \tfrac{1}{2}\eta^2, \qquad \text{i.e.,} \qquad u_{xt} = u_{tt} - \tfrac{1}{2}u_{yy}. \tag{6.4.8}$$

This boundary condition absorbs waves more effectively than (6.4.7), and is the most commonly used absorbing boundary condition of the Engquist-Majda type.

As a higher order example, consider the type $(2,2)$ Padé approximant to $\sqrt{1-s^2}$,

$$r(s) = \frac{1 - \frac{3}{4}s^2}{1 - \frac{1}{4}s^2}.$$

Then (6.4.5) becomes

$$\xi\left(1 - \frac{1}{4}\frac{\eta^2}{\omega^2}\right) = \omega\left(1 - \frac{3}{4}\frac{\eta^2}{\omega^2}\right)$$

or

$$\xi\omega^2 - \tfrac{1}{4}\xi\eta^2 = \omega^3 - \tfrac{3}{4}\omega\eta^2, \qquad \text{i.e.,} \qquad u_{xtt} - \tfrac{1}{4}u_{xyy} = u_{ttt} - \tfrac{3}{4}u_{tyy}. \tag{6.4.9}$$

This third-order boundary condition is harder to implement than (6.4.8), but provides excellent absorption of outgoing waves.

Why didn't we look at the Padé approximation of type (4,0)? There are two answers. First, although that approximation is of the the same order of accuracy as the type (2,2) approximation, it leads to a boundary condition of order 4 instead of 3, which is even harder to implement. Second, that boundary condition turns out to be ill-posed and is thus useless in any case (Exercise 6.4.1). In general, it can be shown that the Engquist-Majda boundary conditions are well-posed if and only if $m = n$ or $n+2$—that is, for precisely those approximations $r(s)$ taken from the main diagonal and first superdiagonal in the "Pade table" (L. N. Trefethen & L. Halpern, *Math. Comp. 47* (1986), pp. 421–435).

Figure 6.4.4, taken from Engquist and Majda, illustrates the effectiveness of their absorbing boundary conditions.* The upper-left plot (1A) shows the initial data: a quarter-circular wave radiating out from the upper-right corner. If the boundaries have Neumann boundary conditions, the wave reflects with reflection coefficient 1 at the left-hand boundary (1B) and again at the right-hand boundary (1C). Dirichlet boundary conditions are equally bad, except that the reflection coefficient becomes -1 (1D). Figure 1E shows the type (0,0) absorbing boundary condition (6.4.7), and the reflected wave amplitude immediately cuts to about 5%. In Figure 1F, with the type (2,0) boundary condition (6.4.8), the amplitude is less than 1%.

EXERCISES

▷ *6.4.1. Ill-posed absorbing boundary conditions.*

(a) What is the type (4,0) Padé approximant $r(s)$ to $\sqrt{1-s^2}$?

(b) Find the coefficients of the corresponding absorbing boundary condition for a left-hand boundary.

(c) Show that this boundary condition is ill-posed by finding a mode $u(x,y,t) = e^{i(\omega t+\xi x+\eta y)}$ that satisfies both the wave equation and the boundary condition with $\eta \in \mathbb{R}$, $\operatorname{Im}\xi > 0$, $\operatorname{Im}\omega < 0$. Explain why the existence of such a mode implies that the initial boundary value problem is ill-posed. In a practical computation, would you expect the ill-posed mode to show up as mild or as explosive?

▷ *6.4.2. Absorbing boundary conditions for oblique incidence.* Sometimes it is advantageous to tune an absorbing boundary condition to absorb not waves that are normally incident at the boundary, but waves at some specified angle (or angles). Use this idea to derive absorbing boundary conditions that are exact for plane waves traveling at 45° in the southwest direction as they hit a left-hand boundary:

(a) Type (0,0), *(b)* Type (2,0).

Don't worry about rigor or about well-posedness. This problem concerns partial differential equations only, not finite difference approximations.

* This figure will appear in the published version of this book only with permission.

Figure 6.4.4. Absorbing boundary conditions for $u_{tt} = u_{xx} + u_{yy}$ (from Engquist & Majda).