Boundary Tracing Methods for Partial Differential Equations

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Abstract

Boundary tracing is a technique that has been used in an ad hoc manner by several authors in their investigations of PDE behaviour [1, 20, 22]. In this thesis a general framework for the technique is developed for two dimensional second order PDEs. Interesting aspects are illustrated through an extensive collection of simple examples.

Boundary tracing is then used to derive new results for a variety of PDEs, including the derivation of new domains admitting exact solutions for the non-linear Laplace–Young equation. These new domains are the only known examples with corners. As such they provide new and verify known results regarding corner behaviour. New results regarding rough surfaces and smooth corners are developed.

Extensions of boundary tracing to higher dimensions and higher order equations are also discussed.
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CHAPTER 1

Introduction

Standard techniques for solving PDEs in two dimensions typically seek out a solution in domains with boundary conditions, both specified \textit{a priori}. Boundary tracing is conceptually different, using a known solution to a PDE to construct new domains in which given boundary conditions are satisfied.

Boundary tracing has been used as an \textit{ad hoc} technique by a few authors [1, 21, 22], as discussed in Chapter 2, however there has been no systematic investigation of its potential.

Normal techniques require simple geometry or are either approximate or numerical for irregular geometry. Boundary tracing leads to exact solutions in non-standard domains. While the technique does not lead to solutions in arbitrary domains, a rich variety of domains can be obtained. These are produced by patching together pieces of boundary to form interesting domains, or through judicious choice of the original PDE solution (\textit{e.g.} using superposition for linear PDEs.)

An important aspect of boundary tracing is that it is insensitive to the nature of the PDE, being equally applicable to linear and non-linear PDEs. Consequently boundary tracing can be used to derive solutions that would be difficult or impossible to obtain using traditional methods. For example, the use of boundary tracing on one of the few known exact solutions to the Laplace–Young equation with the standard contact condition, reveals an infinite family of domains with the same solution; a result of considerable interest. A similar result for Helmholtz's equation can be seen in Example 1.

\textbf{Example 1.} The solution to Helmholtz's equation in the half-plane $y > 0$, with boundary condition $\nabla \eta \cdot \hat{n} = 1$ on $y = 0$ (with $\hat{n}$ being the outward facing normal) is $\eta = e^{-y}$. Boundary tracing reveals that the family of curves given by $y = \ln(\cos(C \pm x))$ for arbitrary $C$ and $-\pi/2 < C \pm x < \pi/2$ also satisfy $\nabla \eta \cdot \hat{n} = 1$ for $\eta = e^{-y}$, which can be verified directly. Additionally, we can patch together several of these curves to generate new domains such as $y > Y(x)$ where $Y(x)$ is defined piecewise as

$$Y(x) = \begin{cases} 0 & x \leq -1 \\ \ln(\cos(1 + x)) & -1 < x \leq 0 \\ \ln(\cos(1 - x)) & 0 < x \leq 1 \\ 0 & 1 < x \end{cases}$$

(1.1)

This domain is shown in Figure 1.1. Thus we have a known solution in a new
domain with a corner. This example will be looked at in greater detail in Chapter 5.

![Figure 1.1](image)

Figure 1.1: A new domain $y > Y(x)$ with $\nabla \eta \cdot \hat{n} = 1$ on the boundary $y = Y(x)$.

Example 1 raises a variety of questions. There are questions particular to the example, such as "Why should we be interested in these new boundaries?" and "Are the boundaries sensible physically?". There are also more general questions, "How can we find such boundaries?", "What boundary conditions can we deal with?", "How do these boundaries behave?" and "What flexibility do we have in constructing domains?".

These are the kinds of questions this thesis attempts to answer. In particular this research investigates boundary tracing in a general context, aiming to provide a coherent framework for its use and to establish the utility of the technique through a variety of examples. These examples include new results for the Laplace-Young capillarity equation.

### 1.1 What is Boundary Tracing?

Boundary tracing is conceptually simple and has simple definition:

**Boundary Tracing**: Given a base function, which is a known exact solution to the PDE of interest over some domain $\Omega \subset \mathbb{R}^2$, boundary tracing means finding one or more curves\(^1\) in $\Omega$, forming the boundary of a new domain, along which prescribed boundary conditions hold.

Typically the boundaries are found by solving a first order ODE associated with the boundary condition, hence the use of the word "tracing".

Whilst the procedure is "an obvious one", it is not obvious that it can be used to construct interesting and useful domains. From these new domains it is sometimes possible to extract information about the general behaviour of solutions.

\(^1\)If $\Omega \subset \mathbb{R}^n$ then the "curve" is an $n-1$ dimensional manifold in $\mathbb{R}^n$. This will be examined in Chapter 8.
1.1. What is Boundary Tracing?

Boundary tracing can also be viewed as solving an inverse problem. *Given that we know the solution and the boundary conditions, where is the boundary?* Often there is no unique solution to this question. It is precisely this non-uniqueness that allows the boundary tracing technique to generate interesting domains. Boundary tracing is most useful when the inverse problem admits infinitely many solutions, rather than having isolated or unique solutions. This occurs with many common boundary conditions, most notably flux type boundary conditions of the form $\nabla \eta \cdot \hat{n} = F$.

The important feature of boundary tracing is that it yields new domains in which *exact* solutions of PDEs, linear or non-linear, exist. Traditional analytic techniques typically result in exact solutions only for certain PDEs in special domains. Approximate techniques are often required to extract results in other cases. The few available exact solutions for non-linear PDEs are of major importance because of their rarity and because such solutions yield information that cannot be readily or reliably extracted using approximate methods. Boundary tracing can sometimes be used with such an exact solution to generate further domains, with exact boundary, in which we have the same exact solution of the PDE.

Although not widely used, the method of boundary tracing has been applied successfully as an *ad hoc* technique in a range of areas to determine physically important results, see Section 2.2. In all of these cases the required boundaries were obtained numerically, whereas for many of the cases presented in this thesis, exact analytic descriptions of the boundary are obtained. Problems of numerical accuracy and convergence don’t arise for these exact solutions and theoretical issues can be more easily addressed.

The extension of these techniques to $N$-dimensional domains results in a PDE for tracing the boundary rather than an ODE. Higher dimensional extensions will be considered in Chapter 8. Three dimensional cases have been examined in the past [19, 21, 22], typically by reducing the problem to two dimensions.

We will see that for higher order PDEs or systems of PDEs in $\mathbb{R}^2$, boundary tracing fails. The difficulty is associated with having more than one boundary condition on the boundaries. Further details are given in Chapter 8. We will also see that in higher dimensions, higher order equations can be accommodated.

Boundary tracing makes no direct reference to the PDE (linear or non-linear); only the solution $\eta$ is directly used by the procedure. Consequently even complicated PDEs admitting sufficiently simple solutions may provide analytic results.

There is limited control over the shape of the domains generated using boundary tracing, as the geometry of the possible traced boundaries is strongly controlled by
the boundary condition and the base function. For linear PDEs infinite sets of base functions are available, so that by judicious choices of these, boundaries of almost any prescribed shape can be generated, (see Chapter 7 for examples.) For non-linear PDEs, typically only isolated solutions exist so the choice of base functions is very restricted, but interesting and useful shapes may still be generated by combining pieces of traced boundaries, see Chapters 4 and 6.

Although it is not always possible to obtain an exact analytic description for the traced boundary curves, important properties can often be extracted directly from the tracing equations. In other situations a numerical representation may suffice. Exact solutions are likely if the PDE solution is highly symmetric and the boundary conditions are also sufficiently simple, see Section 3.5. Note that the new domains do not share these symmetries. As a result of this we may have a radially symmetric \( \eta \) in a non-symmetric domain.

1.2 Overview

As the aims of this project are to both investigate boundary tracing as a technique and establish its utility, this thesis can be considered as several distinct parts: “Motivation” (Chapter 2), “Theory” (Chapter 3), “Examples and Applications” (Chapters 4–7) and “Extensions” (Chapter 8).

Chapter 2 (“Motivation”) describes past uses of boundary tracing and how boundary tracing came to be investigated.

Chapter 3 (“Theory”) describes the general procedure and derives results concerning the shape of boundaries generated by boundary tracing.

“Examples and Applications” begins in Chapter 4, with simple examples of the use of boundary tracing. These examples serve several important purposes:

1. They demonstrate the technique in relatively simple contexts.
2. They show that boundary tracing produces sensible results, by verifying some well known results.
3. They produce several other minor new results.

Most of the examples covered in Chapter 4 are without an associated PDE context. These include \( \eta = (x^2 + y^2)/2 \), \( \eta = xy \), a case where the boundaries are restricted to a bounded region and \( \eta = \sin \rho x \sin \mu y \). Also two PDE examples are considered in depth: Poisson’s equation and the constant mean curvature equation.

The application of boundary tracing to Helmholtz’s equation is examined in Chapter 5 and the Laplace–Young capillarity problem in Chapter 6. In both chapters we derive new domains with corners. Whereas for the Helmholtz’s equation this
is interesting, for the Laplace–Young equation it is significant as there are very few (only 3) exact solutions and no previous exact solutions in domains with corners. These domains are then used to examine many aspects of the behaviour of a solution near a corner and also verify existing results. These chapters also look at approximating rough surfaces using boundary tracing, leading to an explicit relationship between roughness and effective boundary conditions.

Helmholtz’s equation and the Laplace–Young equation are returned to in Chapter 7 where the effect of smoothing a sharp corner is investigated. The derived results are mostly for Helmholtz’s equation with some extensions to the Laplace–Young equation. The most significant result is that for both the Laplace–Young and Helmholtz’s equation “small scale” corner rounding tends to lower the surface height throughout the solution domain, while “large scale” rounding tends to raise the height everywhere.

Extensions of the technique to higher dimensions and higher order PDEs are discussed in Chapter 8. In these cases special difficulties arise that are not encountered in the two dimensional second order case.

The results of the thesis are compiled and discussed in Chapter 9. It is concluded that boundary tracing is a simple and useful technique for investigating PDE behaviour.

Appendix A details some of the numerical methods used to determine traced boundaries, and the methods for generating some of the images.

Appendix B contains the definition of the elliptic integrals that appear repeatedly in the solution of various problems.

Several of the figures in this thesis are complex, with colour versions supplied in Appendix C.
Chapter 1. Introduction
CHAPTER 2

Background

This chapter details how boundary tracing arose in the examination of the Laplace—Young equation and why boundary tracing is worth investigating further. Earlier applications of the technique by other authors are described, demonstrating its versatility.

2.1 How this Research Began

The research behind this thesis began as an investigation of the effects of corner rounding on behaviour of solutions to the Laplace—Young equation in a wedge.

Initial investigations on corner rounding were carried out on Helmholtz’s equation, a small amplitude approximation to the Laplace—Young equation. Problems arose which suggested that simple asymptotic techniques would not work.

An alternate approach was attempted; investigating whether perturbing the solution, \( \eta \), would change the boundary shape in a predictable way. It was then realised that the problem of finding the modified boundary had infinitely many solutions. In fact there was an infinite number of boundaries satisfying the original un-perturbed problem, with the original wedge boundary being the union of two pieces of these boundaries.

A critical discovery was the existence of a single smooth curve that was symmetric about the axis of symmetry of the wedge and satisfied the unperturbed problem. This will be seen in Example 2 and examined in further detail in Chapter 7.

Example 2: The solution to Helmholtz’s equation in the quarter plane with the boundary condition \( \nabla \eta \cdot \hat{n} = 1 \) is \( \eta = e^{-x} + e^{-y} \). Looking at \( \nabla \eta \) along the line \( L : x = y \) we see that at the origin \( ||\nabla \eta|| = \sqrt{2} \), and moving away from the origin \( ||\nabla \eta|| \to 0 \). From this we conclude that there must be some point, \( P = (\ln(\sqrt{2}), \ln(\sqrt{2})) \), on the line L where \( ||\nabla \eta|| = 1 \). Since, by the symmetry of \( \eta \), \( \nabla \eta(P) \) is parallel to \( L \), a piece of curve perpendicular to the line at \( P \) would have \( \nabla \eta \cdot \hat{n} = 1 \). It then seems reasonable that this piece of curve could be extended to give a new curve along which the boundary conditions hold. This curve can be calculated numerically and is shown in Figure 2.1. This traced boundary resembles a quarter plane with rounded corner. Denoting this curve \( Y(x) \), we have an exact solution to Helmholtz’s equation in the domain \( y > Y(x) \), with the domain asymptotically approaching a quarter plane for large \( x \) and \( y \) but having a smoothed corner near the origin.

Other curves satisfying the boundary conditions also exist and are shown in Figure 2.2.
Chapter 2. Background

Figure 2.1: The symmetric traced boundary for Helmholtz's equation in a quarter plane

Figure 2.2: The traced boundaries for Helmholtz's equation in a quarter plane

The extension of these techniques to other angles and other radii of curvature required a more rigorous approach, resulting in the development of some of the general results of Chapter 3.

Searches for new boundaries in cases with stronger symmetry led to exact boundaries for the 1-D solutions for Helmholtz's equation and the Laplace-Young equation. These are examined in Chapters 5 and 6 respectively.

These investigations revealed two general features:

- The technique produced interesting and often surprising results.
- The method could be easily generalised to other geometries and boundary conditions.

These prompted a more complete investigation of the procedure, named boundary tracing, in other contexts.
2.2 Past Examples of Boundary Tracing

Boundary tracing has similarities to other well known techniques such as "thin-wing" aerofoil theory and inverse problems. However the approach employed is distinctly different.

The technique has been successfully used by a number of people in quite different contexts. However, obtaining a proper history of its use is virtually impossible as it has been used only as an *ad hoc* technique. Consequently the following examples should not be considered a comprehensive list of where the technique has been used, merely as evidence that the technique is known and versatile.

To the best of the author’s knowledge this thesis represents the first systematic investigation of the technique.

2.2.1 Growing Roots In a 1969 paper [1] Anderssen, Hale and Radok investigated the ion uptake of a growing single tap root by determining the shape of the “root hair envelope” as a function of time for such roots.

Assuming radial symmetry the authors obtained an approximate description for a curve $C: r = r(z)$ generating this envelope. To do this they first obtained the ion concentration, $C$, due to a combination of sinks moving from $z = 0$ along the $z$ axis. The root hair envelope was then identified as being the location where the Robin condition

$$\nabla C \cdot \hat{n} = kC \quad (2.1)$$

was satisfied, thus defining the curve $C$. The curves were then obtained numerically.

Various existence properties were also proved for the root boundary using two bounding curves for the single sink case. In the paper’s conclusion it was noted that it would only be a minimal increase in the work to obtain numerical results for more realistic non-linear boundary conditions rather than the linear ones considered.

This is an example of an application of the tracing technique for a linear PDE in a 2D context where approximate results were obtained numerically.

2.2.2 Freezing of Ellipsoids A useful measure of the heating or cooling time for an object in a constant temperature environment is the *mean action time* $\Phi(x)$ of the object. The theory for this procedure is given by McNabb [18] and McNabb and Wake [20], and will not be described here. It suffices to note that $\Phi(x)$ satisfies Poisson’s equation

$$\nabla^2 \Phi = -1 \quad (2.2)$$
in the interior of the object and with homogeneous boundary conditions corresponding to the surface conditions under consideration. The maximum value for $\Phi$ in the domain then determines the heating or cooling time. Using this procedure McNabb, Wake, and Anderssen [22] examined the cooling times of ellipsoidal objects with Newtonian surface cooling. This led to the problem of determining $\Phi$ satisfying Poisson's equation with the Robin conditions

$$\Phi + \beta \nabla \Phi \cdot \hat{n} = 0$$

They noted that for the $\beta = 0$ case there is an exact solution given by

$$\Phi = A \left(1 - \frac{x^2}{a^2} - \frac{y^2}{b^2} - \frac{z^2}{c^2}\right),$$

where $A = (a^{-2} + b^{-2} + c^{-2})^{-1}$.

Since there is no known exact solution for ellipsoids in the $\beta \neq 0$ case, they looked for shapes similar to the ellipsoids with the same $\Phi(x)$ obtained for the $\beta = 0$ case. That is, they used boundary tracing. These surfaces were referred to as pseudo ellipses.

It was found that there are infinitely many surfaces satisfying the boundary condition for a particular $\beta$, but they were able to prove that just one of these surfaces has continuous well defined normals everywhere; the rest having corners. The existence of rough surfaces, that is boundaries with arbitrarily small, sharp ridges, satisfying the boundary conditions was also noted. Bounds were obtained for the shape of the smooth pseudo-ellipsoids which were then proven to be very close to ellipses in the two dimensional case. Approximations to the surfaces were generated numerically.

This is again an example of the use of boundary tracing in a linear PDE case (Poisson's equation) where results are extracted numerically but bounds could be established concerning the surface shape. Notably the problem is three dimensional but was solved in two. The presence of rough and non-smooth boundaries rejected in context is also noteworthy. It will be seen that the existence of such boundaries is a regular feature of boundary tracing and in the contexts examined in this thesis these boundaries are of interest.

2.3 Conclusion

Boundary tracing is a novel technique, which has been used to produce new and interesting results. Having been used only in an ad hoc manner it warrants further, more thorough, investigation.
CHAPTER 3

Boundary Tracing

In this chapter we derive results concerning the geometry of boundaries generated by boundary tracing in two dimensions. As the shape of a traced boundary depends only on the boundary condition and the base function \( \eta \), many features of the boundaries can be investigated without direct reference to a PDE.

Boundary existence, direction and curvature are all investigated. The results obtained are especially important when boundary tracing is theoretically possible but the boundaries cannot be obtained analytically. The results are for flux boundary conditions of the general form \( \nabla \eta \cdot \mathbf{n} = F \). These are then specialised to certain boundary conditions. Specifically Dirichlet\(^1\), Neumann, Robin and constant contact angle boundary conditions are examined. We then obtain explicit analytical results for the boundaries when \( \eta \) and the boundary condition have a variety of special symmetric forms\(^2\). Finally we examine the local behaviour of a boundary near certain kinds of singularities of \( \eta \).

3.1 General Flux Boundary Condition

Here we consider the “general flux” boundary condition

\[
\nabla \eta \cdot \mathbf{n} = F
\]  

(3.1)

where \( \mathbf{n} \) is the outwards unit normal to the domain and \( F \) depends only on position, \( \eta \) and \( \eta \)'s derivatives\(^3\).

This is a general boundary condition subsuming a great many common boundary conditions, including homogeneous and non-homogeneous Neumann, Dirichlet and Robin conditions. General flux conditions also include the constant contact angle boundary condition of importance in surface tension problems. These will all be examined in greater detail in Section 3.4.

Boundary tracing looks for curves satisfying a given boundary condition for given \( \eta \). First we identify the the parts of the domain where curves satisfying the boundary condition exist. The direction of these boundary curves is then calculated.

We then look at a variety of details about curve behaviour, finishing with interpreting the boundaries as curves on a smooth manifold. This leads to the unification

\(^1\)Although constant Dirichlet conditions can be dealt with by taking \( F = ||\nabla \eta|| \) they also lead directly to algebraic equations.

\(^2\)These special boundary conditions include the boundary conditions mentioned earlier.

\(^3\)Compare with the \( \nabla \eta \cdot \mathbf{n} \) term, which also depends upon the boundary normal.
of many of the earlier results and provides a geometrical understanding of the more difficult aspects of boundary behaviour.

3.1.1 Viable Domains and Terminal Curves Clearly the boundary condition $\nabla \eta \cdot \hat{n} = F$ cannot be satisfied by any normal direction if $\|\nabla \eta\| < |F|$. This condition divides the domain into two different pieces: The viable domain where $\|\nabla \eta\| \geq |F|$ and the non-viable domain where $\|\nabla \eta\| < |F|$. The boundary between these domains is the terminal curve, where $(\nabla \eta)^2 - F^2 = 0$.

The boundaries between the viable and non-viable domains are called the terminal curves as traced boundaries may begin/end on them. Further details about the behaviour near terminal curves will be given in Subsection 3.1.5.

Introduction of the function $\Phi = (\nabla \eta)^2 - F^2$ simplifies many calculations. The terminal curves are given by $\Phi = 0$ and viable domain by $\Phi > 0$. In addition, the boundary condition can be rewritten as $(\nabla \eta \cdot \hat{r})^2 = \Phi$ where $\hat{r}$ is the unit tangent to the boundary.

3.1.2 Boundary Direction The boundary direction through any point in the viable domain is easily extracted using a local coordinate system based on $\nabla \eta$. Assuming $\nabla \eta \neq 0$, we can expand the unit normal, $\hat{n}$, and unit tangent, $\hat{r}$, of any curve in terms of $\nabla \eta$ and $Q \nabla \eta$, where $Q$ is the linear operator giving rotation by $\pi/2$.

Taking $\alpha$ as the angle between $\hat{n}$ and $\nabla \eta$ we can write $\hat{n}$ and $\hat{r}$ as

$$\hat{n} = \cos \alpha \frac{\nabla \eta}{\|\nabla \eta\|} + \sin \alpha \frac{Q \nabla \eta}{\|\nabla \eta\|}$$

$$\hat{r} = \sin \alpha \frac{\nabla \eta}{\|\nabla \eta\|} - \cos \alpha \frac{Q \nabla \eta}{\|\nabla \eta\|}$$

Now $\nabla \eta$ and $Q \nabla \eta$ are orthogonal, so for any curve satisfying the boundary condition (3.1) we have

$$\nabla \eta \cdot \hat{n} = \cos \alpha \|\nabla \eta\| = F$$

Thus

$$\cos \alpha = F/\|\nabla \eta\|$$

This can be interpreted geometrically using the angle, $\theta$, between $\nabla \eta$ and the tangent to the boundary giving

$$\sin \theta = F/\|\nabla \eta\|$$
3.1. General Flux Boundary Condition

Both $\alpha$ and $\theta$ can be seen in Figure 3.1.

At a point in the viable domain $||\nabla \eta|| \geq |F|$. Provided $||\nabla \eta|| \neq 0$ it is evident that $-1 \leq F/||\nabla \eta|| \leq 1$. Thus the following cases can occur:

1. $-||\nabla \eta|| < |F| < ||\nabla \eta||$ and $F \neq 0$: There are two distinct solutions to (3.5), $\pm \alpha$.

2. $F = \pm ||\nabla \eta||$: These are points on the terminal curve. In this case $\cos \alpha = \pm 1$.
   Thus there is only one solution for $\alpha$. This is $\alpha = 0$ if $F = ||\nabla \eta||$ and $\alpha = \pi$ if $F = -||\nabla \eta||$. Both require $\hat{n}$ to be parallel to $\nabla \eta$, consequently the boundary is locally parallel to the contours of $\eta$.

3. $F = 0$: Then $\cos \alpha = 0$ giving two solutions, $\alpha = \pm \pi/2$. In both cases $\hat{n}$ is perpendicular to $\nabla \eta$, so the boundary is locally perpendicular to the contours of $\eta$.

From (3.2), (3.3) and (3.5), we can obtain two values for the unit tangent and normal to the curve

$$\hat{\tau} = \frac{1}{(\nabla \eta)^2} \left( \mp \sqrt{(\nabla \eta)^2 - F^2} \nabla \eta + FQ \nabla \eta \right) (3.7)$$

$$\hat{n} = \frac{1}{(\nabla \eta)^2} \left( F \nabla \eta \pm \sqrt{(\nabla \eta)^2 - F^2} \nabla \eta \right) (3.8)$$

Earlier we assumed that $\nabla \eta \neq 0$. What happens if this assumption is not true? Then if $F = 0$, $\nabla \eta \cdot \hat{n} = F$ is satisfied by all boundary directions. If $F \neq 0$, then $||\nabla \eta|| < |F|$, so the point does not fall inside the viable domain.

The difficulties arising from the direction field being double valued can be overcome by projecting one of the branches onto the upper half of an appropriate man-

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Figure 3.1: The angles between $\nabla \eta$ and $\hat{n}$ and $\hat{\tau}$ are $\alpha$ and $\theta$ respectively.
Chapter 3. Boundary Tracing

ifold and the other branch onto the lower half. This will be examined in Section 3.3.

3.1.3 The Boundary Tracing ODE Assuming a parametrisation of the boundary\(^5\) of the form \(x = x(t)\) and \(y = y(t)\) we can write the boundary condition (3.1) as

\[
\frac{\eta_x \dot{y} - \eta_y \dot{x}}{\sqrt{\dot{x}^2 + \dot{y}^2}} = \pm F
\]

(3.9)

where we are free to impose an additional constraint to determine the exact parametrisation. (e.g. \(\dot{x}^2 + \dot{y}^2 = 1\) ensures arc-length parametrisation or \(\dot{x} = 1\) is equivalent to using \(y(x)\).) A judicious choice of the parametrisation can greatly simplify the process of determining the curve. In particular the "natural" parametrisation \(t = \eta\) often leads to exact results.

The form of this equation for a variety of common boundary conditions is examined later. Also in Section 3.5 we will see that if \(\eta\) and \(F\) have appropriate symmetry then (3.9) will be integrable.

3.1.4 Ordinary and Critical Points The points in the viable domain can be divided into three types, ordinary points, critical points and terminal points.

Terminal points are points that fall on the terminal curve. Clearly the position of the terminal curves will play an important role in the global behaviour of traced boundaries. Since we already know a little about the terminal curves let us look at critical points.

We define a simple critical point to be a point in the viable domain where all normal directions satisfy the boundary condition (3.1). Taking \(\dot{x} = \cos \phi\) and \(\dot{y} = \sin \phi\) in (3.9), where \(\phi\) is arbitrary, we obtain

\[
\eta_x \sin \phi - \eta_y \cos \phi = \pm F
\]

(3.10)

This can only hold for all \(\phi\) if \(\eta_x = 0, \eta_y = 0\) and \(F = 0\). Thus simple critical points can only occur where \(\nabla \eta = 0\) and \(F = 0\), as was seen in Subsection 3.1.2. It is interesting to note that many boundary conditions have \(F \neq 0\) everywhere, removing the possibility of simple critical points.

\(^5\)Whilst a two dimensional curve can be described either implicitly, as a level curve of some function \(g(x, y)\), or parametrically, as \((x, y) = (x(t), y(t))\), we will use the parametric form.

Looking for boundary curves in the implicit form leads to a PDE for \(g(x, y)\), whereas looking for the curves in the parametric form leads to an ODE for \((x(t), y(t))\). While the two descriptions are equivalent (and in fact identical with the appropriate parameter choice), the parametric description is somewhat easier to work with and will be adopted here.
3.1. General Flux Boundary Condition

The other possible critical points are non-simple ones. These are where either \( \nabla \eta \) or \( F \) has some kind of singularity. The critical points occurring at various types of singularity of \( \eta \) will be examined in Section 3.6.

All other points in the viable domain are ordinary points\(^6\).

3.1.5 Behaviour Near a Terminal Curve

Here we examine the local behaviour of a traced boundary beginning or ending on a terminal curve. Through each point on the terminal curve there are usually two boundaries sharing a common tangent creating a cusp, see Figure 3.3.

Using \( x = t \) as the parametrisation\(^7\), (3.9) can be rearranged to give the ODE

\[
\frac{dy}{dx} = \frac{\eta_x \eta_y \pm F \sqrt{\eta_x^2 + \eta_y^2 - F^2}}{\eta_x^2 - F^2}
\] (3.11)

It is convenient to introduce the function \( \Phi = \eta_x^2 + \eta_y^2 - F^2 \). Near the terminal curve \( \Phi \approx 0 \) so \( \eta_x^2 - F^2 \approx -\eta_y^2 \). Equation (3.11) can be approximated by

\[
\frac{dy}{dx} = -\frac{\eta_x}{\eta_y}
\] (3.12)

Rearranging this gives \( \frac{d\eta_y}{dx} = 0 \). That is, the traced boundaries near the terminal curve are simply contours of \( \eta \) to first order. This result was also shown in Subsection 3.1.2.

The angle, \( \psi \), between the traced boundary and the terminal curve is given by

\[
\cos \psi = \hat{n} \cdot \hat{N} = \frac{\nabla \Phi \cdot \nabla \eta}{\|\nabla \Phi\| \|\nabla \eta\|}
\] (3.13)

where \( \hat{n} \) is a normal to the traced boundary and \( \hat{N} \) is the normal to the terminal curve.

Provided the boundary curve is not tangential to the terminal curve the contours of \( \eta \) cross the terminal curve. However the boundary curves cannot enter the non-viable domain and so must end on the terminal curve, causing a cusp. To better observe this behaviour more terms in the expansion for \( \Phi \) are needed\(^8\). In particular

\(^6\)This definition of an ordinary point may seem “wrong” as typically an ordinary point for boundary tracing will have two solution curves through it, while an ordinary point of an ODE has only one. This definition makes more sense when we consider the direction field as having separate branches. Then an ordinary point is “ordinary”, in the ODE sense, on each of the branches.

\(^7\)We can rotate the coordinate system so that this parametrisation is sensible.

\(^8\)Technically we should expand \( \eta_x, \eta_y \) and \( F \) locally within (3.11), but only the terms under the square-root will contribute to our final expansion as they are of magnitude \((x^{1/2}, y^{1/2})\) whilst the other terms are of order \((x, y)\) and higher.
using a locally centered coordinate system we have \( \Phi = \eta_x^2 + \eta_y^2 - F^2 = ax + by + \ldots \)
where \( a = 2(\eta_x^0 \eta_{xx} + \eta_y^0 \eta_{xy} - F_0 F_x^0) \) and \( b = 2(\eta_x^0 \eta_{xy} + \eta_y^0 \eta_{yy} - F_0 F_y^0) \), where for any symbol \( X, X^0 \) represents \( X(0,0) \). Rewriting the ODE (3.11) including terms up to \( \sqrt{x} \) and \( \sqrt{y} \) we obtain

\[
\frac{dy}{dx} = -\frac{\eta_y^0}{\eta_y^0} \pm \frac{F_0}{(\eta_y^0)^2 \sqrt{ax + by}}
\]

(3.14)

Using the change of variables \( u = ax + by \) we obtain the equation

\[
\frac{du}{dx} = A \pm B \sqrt{u}
\]

(3.15)

where \( A = a - b \eta_x^0 / \eta_y^0 \) and \( B = bF / \eta_y^0 \). Using \( \beta = B / A \) we can solve (3.15), giving

\[
A(x - x_0) = \int \frac{du}{1 \pm \beta \sqrt{u}}
\]

(3.16)

Although this equation can be solved exactly, the solution does not emphasise the important characteristics of the boundary behaviour. Since we are interested in the behaviour near \( x = 0, y = 0 \) and \( u \ll 1 \), a binomial expansion in \( \sqrt{u} \) can be used, giving

\[
A(x - x_0) \approx \int 1 \mp \beta \sqrt{u} \, du
\]

(3.17)

\[
= u \mp \frac{2\beta u^{3/2}}{3} + C
\]

(3.18)

Rearranging and noting that the curve must pass through \((0,0)\) we obtain

\[
(u - Ax)^2 = \frac{4\beta^2}{9} u^3
\]

(3.19)

which is the equation for a semi-cubical parabola (in \( u-x \) coordinates) which has a ceratoid cusp\(^9\) at the origin. The cusp remains after converting back into \( x-y \) coordinates.

Solving (3.19) for \( u \) gives

\[
u \approx Ax \pm \frac{2\beta A^{3/2}}{3} x^{3/2}
\]

(3.20)

Using \( u = ax + by \) and solving for \( y \) gives

\[
y \approx -\frac{\eta_x^0}{\eta_y^0} x \pm \frac{2\beta A^{3/2}}{3} x^{3/2}
\]

(3.21)
3.1. General Flux Boundary Condition

Figure 3.2: The two curves $y = -\frac{u^x}{\eta v} x^2 + \frac{2s A^{3/2}}{3} x^{3/2}$ (A) and $y = -\frac{u^x}{\eta v} x^2 - \frac{2s A^{3/2}}{3} x^{3/2}$ (C), both approximating the traced boundary, are tangential to the curve $y = -\frac{u^x}{\eta v} x$ (B). Together the curves (A) and (C) form a ceratoid cusp at the origin.

An example of these curves can be seen in Figure 3.2.

The expansion fails at terminal critical points as the contours of $\eta$ are locally parallel to the contours of $\Phi$. This results in $A$ in (3.15) being zero and hence $\beta$ is undefined.

Thus traced boundaries have ceratoid cusps at all points of the terminal curve which are not terminal critical points, with the tangents at the cusps being tangential to the contours of $\eta$. This can be seen in Figure 3.3.

Figure 3.3: The boundaries (thin) near the terminal curve (thick) form cusps which are tangential to the contours of $\eta$ (dotted)

The behaviour of the traced boundaries near a terminal critical point is highly dependent upon the curvature of the contours of $\eta$ and $\Phi$ through the point, $\kappa_\eta$ and $\kappa_T$ respectively.

$^9$A ceratoid cusp is a cusp where the radius of curvature tends toward zero along both sides of the cusp. For further details see [29].
In particular if $\kappa_\eta > \kappa_T$ then the cusps formed on the terminal curve merge together creating two smooth boundaries through the critical point. On the other hand if $\kappa_\eta < \kappa_T$ then the cusps on either side of the terminal curve point away from each other resulting in no smooth boundaries through the point. These two situations can be seen in Figure 3.4. These results are best established by examining the traced boundaries on an associated manifold, see Section 3.3.

![Figure 3.4: The local behaviour near a critical terminal point depends upon the curvature of the contours of $\eta$, $\kappa_\eta$, and the curvature of the terminal curve $\kappa_T$. Dotted and continuous lines are traced boundaries on different branches of the direction field, the two black lines on the $\kappa_\eta > \kappa_T$ figure are the smooth boundaries through the critical terminal point.](image)

If all points on the terminal curve have traced boundaries touching them tangentially, then the terminal curve itself is also a viable boundary. This is because the terminal curve is the envelope of the boundaries and an envelope of solutions to a first order ODE is also a solution to the ODE. This occurs frequently in cases with strong symmetry.

3.1.6 Boundary Curvature The curvature of a traced boundary can be expressed in terms of various properties of the base function, $\eta$, and the function $F$.

Consider a traced boundary, parametrised by arc-length. The curvature, $\kappa$, is defined by

$$\frac{d\hat{\tau}}{ds} = \kappa \hat{n}$$  \hspace{1cm} (3.22)

Equivalently for planar curves

$$\frac{d\hat{n}}{ds} = -\kappa \hat{\tau}$$  \hspace{1cm} (3.23)
3.1. General Flux Boundary Condition

To obtain \( \kappa \) in terms of known quantities \((F, \eta \) and their derivatives) we differentiate the boundary condition (3.1) along the boundary giving

\[
\frac{d}{ds}(\nabla \eta) \cdot \hat{n} + \nabla \eta \cdot \frac{d\hat{n}}{ds} = \frac{dF}{ds} \tag{3.24}
\]

Now the derivative along the boundary of \( \nabla \eta \) can be written in terms of the Hessian, \( H \), of \( \eta \).

\[
\frac{d}{ds} \nabla \eta = H \hat{\tau} \tag{3.25}
\]

Similarly

\[
\frac{dF}{ds} = \nabla F \cdot \hat{\tau} \tag{3.26}
\]

This gives\(^{10}\)

\[
\hat{n}^T H \hat{\tau} - \kappa \nabla \eta \cdot \hat{\tau} = \nabla F \cdot \hat{\tau} \tag{3.27}
\]

Thus if \( \nabla \eta \cdot \hat{\tau} \neq 0 \) then

\[
\kappa = \frac{\hat{n}^T H \hat{\tau} - \nabla F \cdot \hat{\tau}}{\nabla \eta \cdot \hat{\tau}} \tag{3.28}
\]

Recall that through every point in the viable domain there are two traced boundaries. The two boundaries have different values for \( \hat{n} \) and \( \hat{\tau} \) and consequently different curvatures. The expression fails where \( \nabla \eta \cdot \hat{\tau} = 0 \). This occurs only on the terminal curves.

Consider approaching the terminal curve along a traced boundary not on the terminal curve. Since we are approaching the terminal curve \( \nabla \eta \cdot \hat{\tau} \to 0 \). Unless \( \hat{n}^T H \hat{\tau} - \nabla F \cdot \hat{\tau} \to 0 \) as we approach the terminal curve the curvature is unbounded and the boundary has a cusp where it hits the terminal line, as was mentioned in Subsection 3.1.5. The other terminal points, with \( \nabla F \cdot \hat{\tau} - \hat{n}^T H \hat{\tau} = 0 \), are called critical terminal points. Critical terminal points are also the points where the boundaries are tangential to the terminal curve\(^{11}\).

\(^{10}\)\(x^T\) denotes the transpose of \(x\) and \(x^TMy = x \cdot (My) = (M^Tx) \cdot y\).

\(^{11}\)The normal to the terminal curve can be written as

\[
\hat{N} = \frac{H\hat{n} - \nabla F}{||H\hat{n} - \nabla F||} \tag{3.29}
\]

Now clearly

\[
\hat{N} \cdot \hat{\tau} = \frac{\hat{\tau}^T H\hat{n} - \hat{\tau} \cdot \nabla F}{||H\hat{n} - \nabla F||} \tag{3.30}
\]

Thus \( \hat{\tau}^T H\hat{n} - \hat{\tau} \cdot \nabla F = 0 \) is equivalent to \( \hat{N} \cdot \hat{\tau} = 0 \), which means the traced boundary is parallel to the terminal curve.
To obtain the curvature at a critical terminal point higher derivatives of the boundary condition (3.1) can be used. Differentiating (3.27) with respect to arclength gives

\[
\frac{d}{ds}(\hat{n}^T H \hat{T}) - \frac{d}{ds}(\kappa \nabla \eta \cdot \hat{T}) = \frac{d}{ds}(\nabla F \cdot \hat{T}) \quad (3.31)
\]

\[
\hat{n}^T H \hat{T} + \hat{n}^T \dot{H} \hat{T} + \hat{n}^T \dot{H} \hat{T} - \kappa \nabla \eta \cdot \hat{T} - \kappa \dot{\nabla} \eta \cdot \hat{T} - \kappa \nabla \eta \cdot \dot{T} = \frac{d}{ds}(\nabla F) \cdot \hat{T} + \nabla F \cdot \dot{T} \quad (3.32)
\]

Here \( \dot{X} \) denotes \( \frac{dX}{ds} \). To express \( \dot{H} \) we introduce the fully symmetric tri-linear function \( J \). Application of \( J \) is essentially contraction with the tensor-like object \( \frac{d^3 \eta}{dx_i dx_j dx_k} \).

That is for \( x_1 = x \) and \( x_2 = y \),

\[
J(a, b, c) = \sum_{i,j,k=1}^2 a_i b_j c_k \frac{d^3 \eta}{dx_i dx_j dx_k} \quad (3.33)
\]

and \( a^T \dot{H} b = J(a, b, \hat{T}) \).

Replacing \( \nabla \eta \cdot \hat{T} \) with 0 in (3.32), and rearranging produces a quadratic for \( \kappa \):

\[
\kappa^2 \nabla \eta \cdot \hat{n} + \kappa(2 \hat{T}^T H \hat{T} - \hat{n}^T \hat{n} + \nabla F \cdot \hat{n}) + \hat{T}^T H F \hat{T} - J(\hat{T}, \hat{T}, \hat{n}) = 0 \quad (3.34)
\]

where \( H^F \) is the Hessian of \( F \). This can then be solved easily for \( \kappa \).

Equation (3.34) can be rewritten using the curvature of the contours of \( \eta \) and \( \Phi \) (or equivalently the terminal curve), \( \kappa_\eta \) and \( \kappa_\Phi \) respectively, resulting in

\[
\kappa^2 \| \nabla \eta \| + \kappa(2 \| \nabla \eta \| \kappa_\eta - \frac{\lambda^{-1}}{2}) - \| \nabla \eta \| \left( \frac{\lambda^{-1}}{2} \kappa_\Phi - \kappa_\eta^2 \right) = 0 \quad (3.36)
\]

where \( \nabla \eta = \lambda \nabla \Phi \) as \( \nabla \eta \) is parallel to \( \nabla \Phi \) on the terminal curves. This does not appear to be a great improvement, but this quadratic has discriminant given by

\[
\Delta = 2 \| \nabla \eta \| \lambda^{-1}(\kappa_\Phi - \kappa_\eta) \quad (3.37)
\]

showing that the existence/nonexistence of smooth curves through the terminal critical point depends upon the relative size of these curvatures, as was mentioned in Subsection 3.1.5.

---

12 This is equivalent to calculating the limit of the curvature along a boundary curve using L' Hopital's rule.

13 The curvature of a contour of \( g(x, y) \) is given by

\[
\kappa_g = \frac{(Q \nabla g)^T H_g (Q \nabla g)}{\| \nabla g \|^3} \quad (3.35)
\]
3.2 Piecing Together Boundaries

Often a single traced boundary on its own produces only an uninteresting or aphysical domain. However by piecing together bits of traced boundaries we can construct domains with interesting features. In constructing these domains we have to ensure our choice of interior/exterior is consistent.

The usual convention that the normal to a boundary points away from the interior of the domain is used. Similarly the boundary parametrisation is orientated such that the interior of the domain is on the left. The exterior of domains are shaded in figures for ease of identification. These conventions are shown in Figure 3.5.

Figure 3.5: The boundary orientation and normal direction of a domain.

For the traced boundaries, one side of the boundary is the interior of the domain, the other the exterior. Since the distinction between the two sides is not evident from images of the boundaries alone, we must be careful when joining together pieces of traced boundary.

For example the boundaries shown in Figure 3.6 can be combined to give new boundaries with corners. The two new domains shown in Figure 3.7 have consistent interior, while the two shown in Figure 3.8 do not, as the choice of interior switches as we pass the point O. Equivalently the direction of parametrisation of the curves at O differ.

If we were to construct the domain shown in Figure 3.9 then the boundary condition $\nabla \eta \cdot \hat{n} = F$ would be satisfied on OD, while the condition $\nabla \eta \cdot \hat{n} = -F$ would hold on OC.
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Figure 3.6: Through each point in the viable domain there are two smooth boundaries.

Figure 3.7: Two pieces of boundary curve can be pieced together in a consistent manner to form a new boundary (AOD and BOC).

Notice also that the distinction of interior/exterior will be similar for neighbouring traced boundaries, as is shown in Figure 3.10. This allows for quick identification of the orientation of a large number of boundaries from a single known one.

In conclusion, we cannot piece together the traced boundaries in a completely arbitrary manner and expect to get sensible domains; care must be taken with the directions of the traced boundaries.

3.2.1 Boundary Orientation Near the Terminal Curve Consider two boundary curves, $C_1$ and $C_2$, forming a cusp at the point P on the terminal curve. Then at P the normals to $C_1$ and $C_2$, $\hat{n}_1$ and $\hat{n}_2$ respectively, are parallel due to the nature of the cusp. Since the normals also satisfy $\nabla \eta \cdot \hat{n} = F$ and assuming $F \neq 0$ we must have $\hat{n}_1 = \hat{n}_2$ (rather than $\hat{n}_1 = -\hat{n}_2$). Thus the situation shown in
3.3 Manifold Interpretation

Figure 3.8: Certain choices of boundary segments lead to inconsistencies in the definition of the interior of the domain.

Figure 3.9: The curve COD must have $\nabla \eta \cdot \hat{n} = F$ on OD and $\nabla \eta \cdot \hat{n} = -F$ on CO if $\eta$ is the same as in Figure 3.6.

Figure 3.11 must occur. Although traced boundaries exhibit cusps on the terminal curves, these cusps cannot be used in the construction of domains like that shown in Figure 3.12. This is because the interiors (and equivalently parametrisations) are not consistent across the cusp\textsuperscript{14}. Only at critical terminal points can a consistent boundary be produced. This is shown by considering the traced boundary behaviour on an associated manifold in Section 3.3.

3.3 Manifold Interpretation

Recall that the valid domain is given by $\nabla \eta^2 - F^2 > 0$, and the terminal curve is given by $\nabla \eta^2 - F^2 = 0$. Let us introduce a third dimension, $z$, into the picture. We can form a smooth surface in three dimensions using $z^2 = \nabla \eta^2 - F^2$. We call this the boundary tracing manifold or simply the manifold. The manifold has a point directly above and below each point in the interior of the viable domain, and the

\textsuperscript{14}For a situation like this to occur one of the curves must have $\nabla \eta \cdot \hat{n} = F$, and the other $\nabla \eta \cdot \hat{n} = -F$. 
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Figure 3.10: Neighbouring curves from the same branch of the direction field have similar choices for interior/exterior.

Figure 3.11: Two curves can form a cusp on the terminal curve. At such a point the direction of the boundaries is the same. Thus no sensible domains with $\nabla \eta \cdot \mathbf{n} = F$ can be constructed using this cusp.

terminal curves are the intersection of the surface with the plane $z = 0$. Clearly there is no point on the manifold above/below any point outside the viable domain. This can be seen in Figure 3.13 (See Figure C.1 for colour version).

Now recall that at each point where $F \neq 0$ we have two directions for the tangent field for the boundary tracing. We can project one “branch” of the tangent field onto the top half of the manifold and the other branch onto the lower half of the manifold. The resulting field on the manifold is single valued everywhere except at critical points and critical terminal points. As is shown in Figure 3.14 (See Figure C.2 for colour version), a curve traced on the manifold does not have a cusp on the terminal curve while the corresponding curve traced in the plane does.

Another advantage of the manifold interpretation is that while the geometry of
3.3. Manifold Interpretation

Figure 3.12: For the cusp made from two traced curves at the terminal curve to be used in a domain one half must satisfy $\nabla \eta \cdot \hat{n} = F$ and the other $\nabla \eta \cdot \hat{n} = -F$.

Traced boundaries near a terminal curve is complex in the $x$-$y$ plane, on the manifold it is simple. In particular the cusps at the terminal curve in the $x$-$y$ plane are locally parabolas on the manifold. Critical terminal points become saddle or spiral points depending upon the sign of $\kappa_\Phi - \kappa_\eta$. These results will be shown below.

For any point $x_0$ on the terminal curve, $\nabla \Phi_0 = \nabla \Phi(x_0)$ will be perpendicular to the manifold and $Q \nabla \Phi_0$ will lie in the intersection of the tangent plane to the manifold at $x$ and the $z = 0$ plane. Any point can then be expressed using $X$, $Y$ and $z$ coordinates as

$$x = x_0 + XQ\nabla \Phi_0 + Y\nabla \Phi_0 + z(0, 0, 1) \quad (3.38)$$

This coordinate system can be seen in Figure 3.15. The plane $Y = 0$ is the tangent plane to the manifold at $x_0$.

Locally $\eta$ and the manifold $z^2 = \Phi$ can be expressed using their power series about $x_0$.

$$\eta(x + \delta x) = \eta_0 + \nabla \eta_0 \cdot \delta x + \frac{1}{2} \delta x^T H_\eta \delta x + \ldots \quad (3.39)$$
$$\Phi(x + \delta x) = \Phi_0 + \nabla \Phi_0 \cdot \delta x + \frac{1}{2} \delta x^T H_\Phi \delta x + \ldots \quad (3.40)$$

Expressing these in the new coordinate system gives

$$\eta = \eta_0 + Y \nabla \eta_0 \cdot \nabla \Phi_0 + X \nabla \eta_0 Q \nabla \Phi_0 + \frac{1}{2} \delta x^T H_\eta \delta x + \ldots \quad (3.41)$$
$$z^2 = Y(\nabla \Phi_0)^2 + \frac{1}{2} \delta x^T H_\Phi \delta x + \ldots \quad (3.42)$$
Figure 3.13: The boundary tracing manifold $z^2 = \nabla \eta^2 - F^2$ (denoted M) takes two $z$ values, for each point in the viable domain (V) but none in the non-viable domain (NV). It intersects the $z = 0$ plane at the terminal curve (T). (See Figure C.1 for colour version)

Recall that near the terminal curve the traced boundaries behave like contours of $\eta$. Thus near the terminal curve, the traced boundaries in $x, y, z$ space are given by the intersection of the contours of $\eta$ (extended in the $z$ direction) with the manifold.

We are interested in the behaviour of the traced boundary on the manifold and the manifold is tangential to the $X-z$ plane at $x_0$. As the traced boundary is locally a contour of $\eta$ and lies in the manifold it must satisfy both (3.41) and (3.42). Thus we can eliminate $Y$ from the equations. This is equivalent to projecting the traced boundary onto the tangent plane.

Eliminating $Y$ from (3.41) and (3.42) to first order when $\nabla \eta_0 \cdot \nabla \Phi_0 \neq 0$ and $\nabla \eta_0 \cdot Q \nabla \Phi_0 \neq 0$ gives

$$\nabla \eta_0 \cdot \nabla \Phi_0 z^2 = (\nabla \Phi_0)^2 (d\eta - (\nabla \eta_0 \cdot Q \nabla \Phi_0) \eta)$$

(3.43)

where $d\eta = \eta - \eta_0$. Each value of $d\eta$ determines a contour of $\eta$ which then gives a single traced boundary, and thus a single curve in the tangent plane.

Equation (3.43) is linear in $X$ and quadratic in $z$ (i.e. it is of the form $aX = bz^2 + c$ for some $a$, $b$ and $c$) so the majority of curves through the terminal curve are locally parabolas when viewed on the manifold.

This fails where $\nabla \eta_0 \cdot \nabla \Phi_0 = 0$ or $\nabla \eta_0 \cdot Q \nabla \Phi_0 = 0$. The first of these has the quadratic term in $z$ vanishing. This term is then replaced by a $z^3$ term thus, in
3.3. Manifold Interpretation

Figure 3.14: A traced boundary (A) in the plane with a cusp at the point P on the terminal curve can be considered a smooth curve (B) on the surface \( z^2 = \nabla \eta^2 - F^2 \) (M). (See Figure C.2 for colour version)

In this case, the traced curves are locally \( X = Mz^3 + Nd\eta \). However this case is not particularly interesting physically and will not be examined in any further detail.

The points where \( \nabla \eta_0 \cdot Q\nabla \Phi_0 = 0 \) are critical terminal points. At these points the \( X^1 \) term will be replaced by a \( X^2 \) term. Since \( \nabla \eta_0 \cdot Q\nabla \Phi_0 = 0 \), \( \nabla \eta_0 \) and \( \nabla \Phi_0 \) are parallel so that \( \nabla \eta_0 = \lambda \nabla \Phi_0 \) for some \( \lambda \). Thus the equations for the manifold and contours of \( \eta \) become

\[
\begin{align*}
\frac{d\eta}{Y} &= Y\lambda(\nabla \Phi_0)^2 + \frac{1}{2}\delta x^T H \delta x + \ldots \\
\frac{dz^2}{Y} &= Y(\nabla \Phi_0)^2 + \frac{1}{2}\delta x^T H \delta x + \ldots
\end{align*}
\]

Eliminating \( Y \) to first order gives

\[
\lambda z^2 - d\eta = \frac{\lambda}{2}\delta x^T H \delta x - \frac{1}{2}\delta x^T H \delta x
\]

Now using \( z^2 = Y(\nabla \Phi_0)^2 + \frac{1}{2}\delta x^T H \delta x + \ldots \) we have \( Y \approx uz^2 + wX^2 \) for some \( u \) and \( w \). Thus \( Y \ll \max\{|X|, |z|\} \). Using this we can write (3.46) as

\[
\begin{align*}
\lambda z^2 - d\eta &= \frac{1}{2} X^2(\lambda(\nabla \Phi_0)^T H \Phi_0 (Q \nabla \Phi_0) - (Q \nabla \Phi_0)^T H (Q \nabla \Phi_0)) \\
&= \frac{1}{2} \lambda X^2 \| \nabla \Phi_0 \|^3 \left( (Q \nabla \Phi_0)^T H \Phi_0 (Q \nabla \Phi_0) - (Q \nabla \eta_0)^T H (Q \nabla \eta_0) \right) \\
&= \frac{1}{2} \lambda X^2 \| \nabla \Phi_0 \|^3 (\kappa_\Phi - \kappa_\eta)
\end{align*}
\]
Figure 3.15: A three dimensional coordinate system based on $\Phi$. $Y$ is in the direction of $\nabla \Phi_0$, $X$ is perpendicular to $\nabla \Phi_0$. The plane shown is the tangent plane to the manifold.

This gives the quadratic

$$z^2 - \frac{1}{3} \| \nabla \Phi_0 \|^3 (\kappa_\Phi - \kappa_\eta) X^2 = \frac{d\eta}{\lambda} \tag{3.50}$$

Here $\kappa_\Phi$ is the curvature of the contours of $\Phi$ and $\kappa_\eta$ is the curvature of the contours of $\eta$. It is clear that the nature of the terminal curves depends upon the relative curvatures of $\eta$ and $\Phi$. If $(\kappa_\Phi - \kappa_\eta) < 0$ then on the manifold the traced curves are given by ellipses (higher order terms will typically cause spiral behaviour instead of closed curves). If $(\kappa_\Phi - \kappa_\eta) > 0$ then the traced curves form a saddle point on the manifold. These results support the results of Subsection 3.1.5.

The two different cases can be seen in Figure 3.16, which shows the manifold (checkerboard), the contours of $\eta$ (black curve), their extensions in the $z$ direction (transparent with black edges) and their intersection, the traced boundaries (white curves).

### 3.4 Special Boundary Conditions

The general flux boundary conditions cover many familiar boundary conditions, including the constant Dirichlet, Neumann, Robin and constant contact angle boundary conditions. The results for critical points, boundary curves and terminal curves can be derived for these boundary conditions. This produces many results which will be used in later chapters. It also allows the differences in traced boundary behaviour for various boundary conditions to be seen.
3.4. Special Boundary Conditions

Figure 3.16: The geometry of the traced boundaries on the manifold at a critical terminal point depends on $\lambda(\kappa_\phi - \kappa_\eta)$.

Under most circumstances we can use an appropriate local orthogonal transformation of coordinates to express $\eta$ near an ordinary point as $\eta = Ax + B$ for some $A$ and $B$. These $\eta = Ax + B$ cases determine, to first order, what happens at all ordinary points$^{15}$ so we will examine this simple example for each boundary condition.

In this section the boundary curves are parametrised using some arbitrary parameter $t$, and $\dot{x}$ represents the derivative with respect to $t$, $\frac{dx}{dt}$, rather than the derivative with respect to arclength, $\frac{d}{ds}$.

As many similar results are derived in each subsection the casual reader may wish to skim through this section and refer back later as necessary.

3.4.1 Constant Dirichlet Boundary Conditions Dirichlet boundary conditions,

$$\eta = c$$

(3.51)

occur in many PDE problems. This class of boundary conditions includes the homogeneous Dirichlet condition, $\eta = 0$ as a special case.

When the boundary condition takes this form we have an algebraic equation to solve to obtain the boundary, rather than an ODE. Typically this results in isolated curves as solutions. Changing the value of $c$ leads to new boundaries, forming "shells" in the direction of $\nabla \eta$.

$^{15}$Points outside the viable domain are also transformable to $\eta = Ax + B$, so not all choices of $A$ and $B$ need correspond to an ordinary point.
Although this boundary condition seems to not fit into the class of general flux boundary conditions, considering all choices of \( c \) simultaneously we can derive an equivalent flux boundary condition. The boundary condition \( \eta = c \) means that the value of \( \eta \) does not change along the boundary. Thus, \( \nabla \eta \cdot \hat{T} = 0 \) where \( \hat{T} \) is a unit tangent to the boundary. Now since \( \hat{T} \) and \( \hat{n} \) are perpendicular \( (\nabla \eta \cdot \hat{T})^2 + (\nabla \eta \cdot \hat{n})^2 = ||\nabla \eta||^2 \). Thus the boundary condition can be written

\[
\nabla \eta \cdot \hat{n} = F = \pm ||\nabla \eta|| \tag{3.52}
\]

Now using the results from earlier in this chapter we can see that

1. The boundary curves are perpendicular to the gradient. Consequently the boundary curve is a contour of \( \eta \). Thus through every point in the domain of \( \eta \) where \( \nabla \eta \) is defined and \( \nabla \eta \neq 0 \) there is a single boundary satisfying the boundary condition.

2. In Cartesian coordinates the differential equation that the boundaries must satisfy is

\[
\frac{\eta_x \dot{y} - \eta_y \dot{x}}{\sqrt{\dot{x}^2 + \dot{y}^2}} = \sqrt{\eta_x^2 + \eta_y^2} \tag{3.53}
\]

This can be rearranged to give

\[
\dot{x} \eta_x + \dot{y} \eta_y = \frac{d}{dt} \eta = 0
\]

3. Critical points occur where \( F = ||\nabla \eta|| = 0 \) and \( \nabla \eta = 0 \), so any point where \( \nabla \eta = 0 \) is a critical point for the tracing equations. All other points where \( \nabla \eta \) is well defined are ordinary points.

4. The terminal curves are given by \( (\nabla \eta)^2 - F^2 = 0 \), so we get a degenerate case where the entire domain is a terminal curve. But since we already know that through every point where \( \eta \) is well defined there is at least one curve, we conclude that the notion of the terminal curve has no sensible meaning in this case.

5. The curvature of a boundary at any point with \( \nabla \eta \neq 0 \) is given by

\[
\kappa = \frac{\dot{\hat{T}}^T H \dot{\hat{T}}}{\nabla \eta \cdot \hat{n}} = \frac{\nabla \eta^T Q^T HQ \nabla \eta}{||\nabla \eta||^3} \tag{3.55}
\]

It is easiest to derive this directly from \( \hat{T} \cdot \nabla \eta = 0 \).
3.4. Special Boundary Conditions

Example 3. Consider the base function $\eta = Ax + B$ with the boundary condition is $\eta = c = 1$. It is easy to see that the only valid boundary is the line $x = (1 - B)/A$.

Now considering the whole range of choices for $c$ we obtain a family of lines $x = (c - B)/A$. It is easy to see that these are solutions to $\nabla \eta \cdot \hat{n} = ||\nabla \eta||$.

3.4.2 Homogeneous Neumann Boundary Conditions

Homogeneous Neumann boundary conditions,

$$\nabla \eta \cdot \hat{n} = 0$$

are often used to represent zero flux, or insulating boundaries. These boundary conditions are the general flux conditions, (3.1), with $F = 0$. Consequently the traced boundaries have the following properties:

1. The boundary curves are parallel to the gradient, thus perpendicular to the contours of $\eta$ at every point. This means that there is a single boundary satisfying the boundary condition through every point in the domain of $\eta$ where $\nabla \eta$ is defined and $\nabla \eta \neq 0$.

2. In Cartesian coordinates the differential equation that the boundaries must satisfy is

$$\eta_x(x, y) \dot{y} - \eta_y(x, y) \dot{x} = 0$$

(3.57)

3. Critical points occur where $F = 0$ and $\nabla \eta = 0$, so any point where $\nabla \eta = 0$ is a critical point for the tracing equations. All other points where $\nabla \eta$ is well defined are ordinary points.

4. The terminal curves are given by $(\nabla \eta)^2 - F^2 = 0$, so the only terminal curves are where $\nabla \eta = 0$ (which will usually be only isolated points.) Another way of looking at this is that since a boundary curve is defined through every point where $\nabla \eta$ is well defined it is evident that there are no terminal curves.

5. The curvature of a boundary at any ordinary point is given by

$$\kappa = \frac{\hat{n}^T \hat{\tau}}{\nabla \eta \cdot \hat{\tau}}$$

(3.58)

which reduces to

$$\kappa = \frac{\nabla \eta^T Q^T H \nabla \eta}{||\nabla \eta||^3}$$

(3.59)

since $\nabla \eta$ is parallel to the boundary.
6. There are no terminal curves and hence no critical terminal points.

Not surprisingly the traced boundaries for homogeneous Neumann boundary conditions are orthogonal to the boundaries for Dirichlet boundary conditions.

**Example 4.** Taking \( \eta = Ax + B \) the contours of \( \eta \) are the \( x = \text{const} \) curves. Thus we would expect the curves \( y = \text{const} \) to be the desired boundary curves and this can be verified trivially. These are shown in Figure 3.17.

![Figure 3.17: Boundary tracing for \( \nabla \eta \cdot \hat{n} = 0 \)](image)

### 3.4.3 Constant Non-homogeneous Neumann Boundary Conditions

Non-homogeneous Neumann boundary conditions,

\[
\nabla \eta \cdot \hat{n} = c \tag{3.60}
\]

usually represent constant flux across the boundary. They are the general flux boundary condition with \( F = c \). The traced boundaries have the following properties:

1. The angle \( \theta \), between the boundary and the gradient is given by

\[
\theta = \sin^{-1} \frac{c}{||\nabla \eta||} \tag{3.61}
\]

A graph of \( \theta \) as a function of \( ||\nabla \eta|| \) for \( c = 1 \) can be seen in Figure 3.18.

2. Through every point in the domain of \( \eta \) where \( ||\nabla \eta|| > c \) there are two distinct traced boundaries falling an angle \( \pi/2 - \theta \) on either side of \( \nabla \eta \).

3. If we define the boundary parametrically in rectangular Cartesian coordinates as \( x = x(\rho) \), \( y = y(\rho) \) the boundary condition becomes

\[
\frac{-\dot{y} \eta_x + \dot{x} \eta_y}{\sqrt{\dot{x}^2 + \dot{y}^2}} = \pm c \tag{3.62}
\]
Figure 3.18: $\theta$ vs $\|\nabla \eta\|$ for $c = 1$ with the boundary condition $\nabla \eta \cdot \hat{n} = 1$

4. Since critical points for the general flux boundary conditions can only occur where $F = 0$ or $\nabla \eta$ is undefined, the only critical points for the $\nabla \eta \cdot \hat{n} = c$ occur where $\nabla \eta$ is undefined.

As the gradient becomes large, $\alpha$ approaches $\pi/2$ and the two possible boundary tangents approach the direction of the gradient of $\eta$ from opposite sides.

5. The terminal curves are $\|\nabla \eta\| = |c|$.

6. Boundary curvature away from the terminal curve is

$$\kappa = \frac{-\hat{n}^T H \hat{\tau}}{\nabla \eta \cdot \hat{\tau}}$$  \hspace{1cm} (3.63)

7. The critical terminal points are on the terminal curve $\nabla \eta^2 = c^2$ and have $\nabla \eta$ parallel to $\nabla \Phi = 2H \nabla \eta$, so

$$(Q \nabla \eta) \cdot (H \nabla \eta) = 0$$  \hspace{1cm} (3.64)

This requires $\nabla \eta$ to be an eigenvector of $H$, so $H \nabla \eta = \lambda_1 \nabla \eta$. Since $H$ is symmetric $Q \nabla \eta$ is also an eigenvector of $H$, so $HQ \nabla \eta = \lambda_2 Q \nabla \eta$. Using these results the formula for curvature at a critical terminal point becomes

$$c\kappa^2 + (2\lambda_1 - \lambda_2)\kappa - J(\hat{\tau}, \hat{\tau}, \hat{n}) = 0$$  \hspace{1cm} (3.65)

**Example 5.** Given the base function $\eta = Ax + B$, parametrising our boundary curve using $y = y(x)$ reduces the differential equation (3.62) to

$$-A \frac{\dot{y}(x)}{\sqrt{1 + \dot{y}(x)^2}} = c$$  \hspace{1cm} (3.66)
which, if $|A| > |c|$, has solution
\[
y = \pm \frac{cx}{\sqrt{A^2 - c^2}} + K
\]  
(3.67)

where $K$ is a constant of integration. Note that these equations describe two families of parallel lines like those in Figure 3.19.

Figure 3.19: Solution boundary curves with $\nabla \eta \cdot \hat{n} = c$ when $\eta = Ax$.

### 3.4.4 Homogeneous Robin Boundary Conditions

Robin Boundary conditions of the form
\[
\nabla \eta \cdot \hat{n} = b\eta
\]  
(3.68)

model diffusion across a boundary when the flux is affected by the concentration at the boundary. They are general flux boundary conditions with $F = b\eta$. The traced boundaries have the following properties:

1. $\cos \alpha = \frac{b\eta}{||\nabla \eta||}$
2. The differential equation is
\[
\frac{-\eta_y \dot{x} + \eta_x \dot{y}}{\sqrt{\dot{x}^2 + \dot{y}^2}} = \pm b\eta
\]  
(3.69)

3. The critical points occur where $\eta = 0$ and $\nabla \eta = 0$.
4. The terminal curves are given by
\[
||\nabla \eta||^2 = b^2 \eta^2
\]  
(3.70)
5. The boundary curvature is given by
\[
\kappa = b - \frac{\hat{n}^T H \dot{\hat{r}}}{\nabla \eta \cdot \dot{\hat{r}}}
\]  
(3.71)
3.4. **Special Boundary Conditions**

**Example 6.** Again considering \( \eta = Ax + B \) we obtain

\[
a(Ax + B) + \frac{bA\dot{y}}{\sqrt{1 + \dot{y}^2}} = 0
\]  

(3.72)

Solving for \( \dot{y} \) and defining \( \beta = b/a \) and \( \alpha = -B/A \) and finally integrating gives

\[
y = \pm \int \frac{x - \alpha}{\sqrt{\beta^2 - (x - \alpha)^2}} \, dx = \pm \sqrt{\beta^2 - (x - \alpha)^2} + C
\]

(3.73)

This can be rearranged to give

\[
(y - C)^2 + (x - \alpha)^2 = \beta^2
\]

(3.74)

Thus the solutions are circles with radius \( b/a \) centered on the line \( x = B/A \). Also the terminal curves \( x = B/A \pm b/a \) are solutions as they are the envelope of the circle solutions.

### 3.4.5 Non-homogeneous Robin Boundary Conditions

Non-homogeneous Robin boundary conditions

\[
a\eta + b\nabla \eta \cdot \hat{n} = c
\]

(3.75)

are used in similar situations to the homogeneous Robin conditions. They are general flux boundary conditions with \( F = \frac{c-a\eta}{b} \). The traced boundaries have the following properties:

1. \( \cos \alpha = \frac{c-a\eta}{b\|\nabla \eta\|} \)

2. The differential equation is

\[
\frac{-\eta_x \dot{x} + \eta_y \dot{y}}{\sqrt{\dot{x}^2 + \dot{y}^2}} = \pm \frac{c-a\eta}{b}
\]

(3.76)

3. Critical points where \( \eta = c/a \) and \( \nabla \eta = 0 \).

4. The terminal curves are given by

\[
\|\nabla \eta\|^2 = \frac{(c-a\eta)^2}{b^2}
\]

(3.77)

5. The boundary curvature is given by

\[
\kappa = \frac{\nabla F \cdot \hat{\tau} - \hat{n}^T \mathbf{H} \hat{\tau}}{\nabla \eta \cdot \hat{\tau}}
\]

(3.78)

\[
\frac{a}{b} - \frac{\hat{n}^T \mathbf{H} \hat{\tau}}{\nabla \eta \cdot \hat{\tau}}
\]

(3.79)
Example 7. Using the function $\eta = Ax + B$ and assuming the boundary is of the form $y = y(x)$ the boundary conditions become

$$a(Ax + B) + \frac{bAy}{\sqrt{1 + \dot{y}^2}} = c \quad (3.80)$$

Solving this for $\dot{y}$ gives

$$\dot{y} = \pm \frac{x - \alpha}{\sqrt{\beta^2 - (x - \alpha)^2}} \quad (3.81)$$

As in the previous example the solutions to this equation are circles of radius $\beta = b/a$, this time centered on any point on the line $x = \alpha = \frac{aB - c}{aA}$. It can also be shown that the terminal curves $x = \alpha \pm \beta$ are valid boundaries, as they are the envelope of the other solutions. The solutions are shown in Figure 3.20

![Figure 3.20: Solution boundary curves with $a\eta + b\nabla \eta \cdot \hat{n} = c$ when $\eta = Ax$.](image)

3.4.6 Constant Contact Angle Boundary Conditions These boundary conditions are of the form

$$\frac{\nabla \eta \cdot \hat{n}}{\sqrt{1 + |\nabla \eta|^2}} = \cos \gamma \quad (3.82)$$

The surface $\eta$ meets the boundary cylinder, $\{(x, y, z) : (x, y) \in \partial \Omega\}$, at a specified angle $\gamma$. Another way of interpreting this is that the angle between the surface normal and the boundary normal (in three dimensions) is $\gamma$.

This boundary condition can be rewritten as a general flux boundary condition with $F = \cos \gamma \sqrt{1 + |\nabla \eta|^2}$.

Using the results from Section 3.1 we obtain the following
3.4. Special Boundary Conditions

Figure 3.21: **Plot of** $\alpha = \arccos(\cos \gamma \sqrt{1 + 1/\nabla \eta^2})$ **for** $\gamma = \pi/8, \pi/4, 3\pi/8$. **The horizontal dotted lines are** $\alpha = \pi/8, \pi/4, 3\pi/8$, **the vertical lines** $\|\nabla \eta\| = \cot(3\pi/8), \cot(\pi/4), \cot(\pi/8)$

1. $\cos \alpha = \cos \gamma \sqrt{1 + 1/\nabla \eta^2}$. Thus $\alpha < \gamma$. Also as $\|\nabla \eta\| \to \gamma$, $\alpha \to 0$ and as $\|\nabla \eta\| \to \infty$, $\alpha \to \pm \gamma$. A plot of $\alpha$ against $\|\nabla \eta\|$ can be seen in Figure 3.21.

2. The differential equation for the boundary in Cartesian coordinates is

$$\frac{-\dot{y} \eta_z + \dot{x} \eta_y}{\sqrt{\dot{x}^2 + \dot{y}^2}} = \pm \cos \gamma$$

(3.83)

3. There are no critical points except essential ones as $F > 0$.

4. The terminal curves are

$$\nabla \eta^2 - F^2 = \sin^2 \gamma \nabla \eta^2 - \cos^2 \gamma = 0$$

(3.84)

5. Boundary curvature is

$$\kappa = \frac{1}{\nabla \eta \cdot \hat{\tau}} \left( \frac{\cos \gamma \nabla \eta}{\sqrt{1 + \nabla \eta^2}} \right)^T$$

(3.85)

This can be obtained by substituting $\nabla F = \frac{\cos \gamma \nabla \eta}{\sqrt{1 + \nabla \eta^2}}$ into the equation for curvature.

**Example 8.** Again taking $\eta = Ax + B$ and parametrising the boundary as $y = y(x)$ the differential equation for the boundary, (3.83) becomes

$$\frac{-A}{\sqrt{1 + A^2}} \frac{\dot{y}}{\sqrt{1 + \dot{y}^2}} = \pm \cos \gamma$$

(3.86)
So long as $|A| > |\cot \gamma|$ this can be solved, giving the boundary curves as

$$y = \pm \cot \gamma - \frac{\sqrt{A^2 + 1}}{\sqrt{A^2 - \cot^2 \gamma}} x + K$$  \hspace{1cm} (3.87)

As in Example 5 we again obtain two families of parallel lines, similar to those shown in Figure 3.19.

### 3.5 Symmetric Cases

In certain strongly symmetric cases it is possible to obtain exact equations for the boundaries produced by boundary tracing. We will examine the results of using boundary tracing on rotationally symmetric $\eta$ as well as the case where $\eta$ is a function of $y$ alone. We will also use the results from earlier in this chapter to examine what happens to the curvature of the boundary in these symmetric cases.

These techniques, along with others will be used to examine the behaviour of solutions to various PDEs in later chapters.

In this section we will consider a restricted version of the general flux boundary condition

$$\nabla \eta \cdot \hat{\mathbf{n}} = F(\eta, \|\nabla \eta\|)$$  \hspace{1cm} (3.88)

This set of boundary conditions contains all those from Section 3.4.

#### 3.5.1 The One Dimensional Case $\eta = \eta(y)$

If $\eta = \eta(y)$ and consequently $\nabla \eta = \eta_y(y) \hat{j}$ then we can write (3.88) as

$$\nabla \eta \cdot \hat{\mathbf{n}} = F(\eta(y), |\eta_y(y)|) = G(y)$$  \hspace{1cm} (3.89)

The terminal curves are given by $\eta_y(y)^2 - G(y)^2 = 0$, which gives a set of lines of the form $y = \text{const}$. These lines satisfy the boundary conditions. The viable domains are bounded by these lines, and are given by $\eta_y^2 > G(y)^2$.

A boundary of the form $y = y(x)$ has normal

$$\hat{\mathbf{n}} = \frac{-y'(x)\hat{i} - \hat{j}}{\sqrt{1 + y'(x)^2}}$$

Requiring that the boundary satisfies the boundary condition (3.89) gives

$$G(y) = \nabla \eta \cdot \hat{\mathbf{n}} = \frac{-\eta_y}{\sqrt{1 + y'(x)^2}}$$

$$\frac{dy}{dx} = \pm \sqrt{\left(\frac{\eta_y(y)}{G(y)}\right)^2 - 1}$$
This can be integrated to give

\[ x = C \pm \int \frac{|G(y)|}{\sqrt{\eta_y(y)^2 - G(y)^2}} \, dy \]  \hspace{1cm} (3.90)

Assuming we can invert the integral we would obtain \( y = f(\pm x + C) \) for some function \( f \). The \( \pm x + C \) means that translating a traced boundary curve in the \( x \) direction will result in a new traced boundary, as will reflection in the \( x \) direction. This is not surprising as \( \eta \) had these same symmetries.

We can also calculate the curvature using the equations in Subsection 3.1.6. Some simple manipulations give us

\[ \kappa = \frac{G'(y)\eta_y - G(y)\eta_{yy}}{\eta_y^2} \]  \hspace{1cm} (3.91)

3.5.2 The One Dimensional Case \( y = y(\eta) \) The case when \( y = y(\eta) \) is the implicit case of Subsection 3.5.1 This technique is useful when we can express the \( y \) coordinate in terms of the solution height \( \eta \), but not the other way around\(^{16}\). Interestingly this leads to simpler parametric equations for the boundary than the earlier method, but eliminating the parameter \( \eta \) is not necessarily easy or even possible.

The boundary condition (3.88) becomes

\[ \nabla \eta \cdot \hat{n} = F(\eta, ||\nabla \eta||) = F(\eta, 1/y'(\eta)) = G(\eta) \]  \hspace{1cm} (3.92)

The gradient of \( \eta \) is given by

\[ \nabla \eta = \frac{1}{y'(\eta)} \hat{j} \]  \hspace{1cm} (3.93)

A boundary solution of the form \( x = x(\eta) \) and \( y = y(\eta) \) has normal

\[ \hat{n} = \frac{y'(\eta)\hat{i} - x'(\eta)\hat{j}}{\sqrt{x'(\eta)^2 + y'(\eta)^2}} \]

If this boundary satisfies the boundary condition (3.92) then

\[ G(\eta) = \hat{n} \cdot \nabla \eta = \frac{-x'(\eta)/y'(\eta)}{\sqrt{x'(\eta)^2 + y'(\eta)^2}} \]

\[ x'(\eta) = \pm \frac{G(\eta)y'(\eta)}{\sqrt{1 - G(\eta)^2y'(\eta)^2}} \]

\(^{16}\)This is the case for the Laplace–Young equation in Chapter 6.
This can be integrated to give
\[ x(\eta) = C \pm \int \frac{G(\eta)y'(\eta)}{\sqrt{1 - G(\eta)^2y'(\eta)^2}} \, d\eta \quad (3.94) \]

This solution is of the form \( y = f(\pm x + C) \) for some \( f \), meaning that we can obtain solutions through translations in the \( x \) direction and reflections in the \( x \) direction.

Using simple manipulations the curvature can be shown to be
\[ \kappa = \frac{y'(\eta)G'(\eta) + G(\eta)y''(\eta)}{y'(\eta)} \quad (3.95) \]

3.5.3 The One Dimensional Case \( \eta_v = g(\eta) \) This case is when the solution is independent of \( x \) and the slope in the \( y \) direction can be expressed as a function of height alone\(^{17}\).

The boundary condition (3.88) becomes
\[ \nabla \eta \cdot \hat{n} = F(\eta, ||\nabla\eta||) = F(\eta, |g(\eta)|) = G(\eta) \quad (3.96) \]

If \( \eta_v = g(\eta) \) then parametrising the boundary using \( x(\eta) \) and \( y(\eta) \) will lead to a solution. Derivatives will be with respect to \( \eta \) unless otherwise noted, i.e. \( \dot{x} \) will be \( \dot{\eta} \).

First \( y(\eta) \) can be shown to be
\[ y(\eta) = \int \frac{dy}{d\eta} \, d\eta = \int \frac{1}{g(\eta)} \, d\eta \]

The boundary condition can be written as the following ODE
\[ \frac{\eta_v \dot{x}}{\sqrt{\dot{x}^2 + \dot{y}^2}} = G \quad (3.97) \]

which after solving for \( \dot{x} \) gives
\[ \dot{x} = \pm \frac{G\dot{y}}{\sqrt{\eta_v^2 - G^2}} \]

Now using \( \eta_v = g(\eta), \dot{y} = 1/g(\eta) \) and integrating we obtain
\[ x = C \pm \int \frac{G}{g\sqrt{g^2 - G^2}} \, d\eta \quad (3.98) \]

This has the same translation/reflection properties as the earlier cases.

The curvature can be shown to be
\[ \kappa = \frac{gG' - g'G}{g} \quad (3.99) \]

\(^{17}\)This is again useful for the Laplace–Young equation in Chapter 6.
3.5.4 The Radially Symmetric Case $\eta = \eta(r)$ For the boundary condition (3.88) we obtain
\[ \nabla \eta \cdot \hat{n} = F(\eta, ||\nabla \eta||) = F(\eta(r), |\eta_r(r)|) = G(r) \] (3.100)
The gradient of $\eta$ is given by
\[ \nabla \eta = \eta_r \hat{e}_r + \frac{1}{r} \eta_\theta \hat{e}_\theta = \eta_r \hat{e}_r \]
where $\hat{e}_r$ is the unit radial vector. Assuming a boundary of the form $r = R(\theta)$, the normal is given by
\[ \hat{n} = \frac{(R(\theta)\hat{e}_r - \dot{R}(\theta) e_\theta)}{\sqrt{\dot{R}(\theta)^2 - R(\theta)^2}} \]
The boundary condition then implies that
\[ \nabla \eta \cdot \hat{n} = G = \frac{R(\theta)\eta_r}{\sqrt{\dot{R}(\theta)^2 - R(\theta)^2}} \]
\[ \frac{dR}{d\theta} = \pm \frac{R}{G} \frac{1}{\sqrt{\eta_r^2 - G^2}} \]
which can be integrated to give
\[ \theta = C \pm \int \frac{G \, dr}{r \sqrt{\eta_r^2 - G^2}} \] (3.101)
In this case, if we can solve the equation for $R$, we obtain $R = f(\pm \theta + C)$ for some $f$. This shows that solutions can be obtained by rotation about the origin or reflection across a line through the origin.

The curvature can be shown to be
\[ \kappa = \frac{r G_r \eta_r + r G \eta_{rr} \eta_r + G}{r \eta_r^2} \] (3.102)

3.6 Behaviour Near Simple Singularities

Exact solutions to PDEs often contain singularities. The position and nature of such singularities strongly influence the behaviour of traced boundaries locally and possibly globally.

In this section we examine the behaviour of boundaries near a simple singularity. Only two simple types of singularities are considered: radial singularities, for example $\eta = 1/r$, and line singularities, such as $\eta = \sqrt{y}$.

There are, of course, other singularities that do not fit into these categories such as $\eta = \sin \theta \sqrt{r}$. Such singularities are not considered here.
3.6.1 Line Singularities

Assuming that near a line singularity at \( y = 0, \eta \) takes the form

\[
\eta = Ay^n
\]  

Then we have a singularity at \( y = 0 \) if \( n < 1 \).

We assume that near \( y = 0 \) we can express the boundary condition as

\[
\nabla \eta \cdot \hat{n} = F = By^\sigma
\]  

for some \( B \) and \( \sigma \).

Since \( \eta \) and \( F \) are functions of \( y \) alone, equation (3.90) of Subsection 3.5.1 can be used, giving

\[
x = C \pm \int \frac{F}{\sqrt{\eta_y^2 - F^2}} \, dy
\]

\[
= C \pm \int \frac{By^\sigma}{\sqrt{A^2\nu^2y^{2\nu-2} - B^2y^{2\sigma}}} \, dy
\]

Clearly we will only have a solution if for \( 0 < y < 1, a^2\nu^2y^{2\nu-2} - B^2y^{2\sigma} > 0 \). This is true when either \( 2\nu - 2 < 2\sigma \) giving

\[
\nu - 1 - \sigma < 0
\]  

or \( 2\nu - 2 = 2\sigma \) and \( a^2\nu^2 - B^2 > 0 \), giving

\[
\nu - 1 - \sigma = 0 \quad \text{and} \quad \left| \frac{B}{A\nu} \right| < 1
\]  

Now if \( \nu - 1 - \sigma = 0 \) (equivalently \( \sigma = \nu - 1 \))

\[
x = C \pm \int \frac{By^{n-1}}{\sqrt{A^2\nu^2y^{2\nu-2} - B^2y^{2\nu-2}}} \, dy
\]

\[
= C \pm \int \frac{B}{\sqrt{A^2\nu^2 - B^2}} \, dy
\]

\[
= C \pm \frac{By}{\sqrt{A^2\nu^2 - B^2}}
\]

Thus the angle, \( \phi \), between the traced boundaries and the line of the singularity is given by

\[
\cos \phi = \frac{B}{A\nu}
\]
3.6. Behaviour Near Simple Singularities

If \( \nu - 1 - \sigma < 0 \) then \( \nu - 1 = \sigma - \epsilon \) for some \( \epsilon > 0 \).

\[
x = C \pm \int \frac{B y^\epsilon}{\sqrt{A^2 \nu^2 - B^2 y^{2\epsilon}}} \, dyanumber{(3.113)}
\]

For \( y \approx 0 \) this becomes

\[
x \approx C \pm \frac{B}{A \nu} \int y^\epsilon \, dy = C \pm \frac{B y^{\epsilon+1}}{A \nu (\epsilon + 1)}anumber{(3.114)}
\]

In this case the boundaries are locally perpendicular to the line of the singularity.

3.6.2 Radial Singularities

Here we assume that the singularity has the form

\[
\eta = Ar^\nu
\]

and that the boundary condition near \( r = 0 \) can be approximated by

\[
\nabla \eta \cdot \hat{n} = F = Br^\sigma
\]

Since \( \eta \) is a function of \( r \) only, equation (3.101) of Subsection 3.5.4 can be used giving

\[
\theta = C \pm \int \frac{F}{r \sqrt{\eta_r^2 - F^2}} \, dr
= C \pm \int \frac{Br^\sigma}{r \sqrt{A^2 \nu^2 r^{2\nu - 2} - B^2 r^{2\sigma}}} \, dr
\]

As in the previous section we will only have solutions to this if \( \nu - 1 - \sigma < 0 \) or both \( \nu - 1 - \sigma = 0 \) and \( \frac{|B|}{A \nu} < 1 \).

When \( \nu - 1 - \sigma = 0 \) then \( \nu = \sigma + 1 \) so

\[
x = C \pm \int \frac{Br^\sigma}{r \sqrt{A^2 \nu^2 r^{2\nu - 2} - B^2 r^{2\sigma}}} \, dr
= C \pm \frac{B \log(r)}{\sqrt{A^2 \nu^2 - B^2}}anumber{(3.120)}
\]

Thus a traced boundary approaching the singularity spirals toward the singularity, making an infinite number of revolutions.

If \( \nu - 1 = \sigma - \epsilon \) for some \( \epsilon > 0 \), then

\[
\theta = C \pm \int \frac{Br^\epsilon}{r \sqrt{A^2 \nu^2 - B^2 r^{2\epsilon}}} \, dr
\]

Since we are only interested in the case where \( 0 < r \ll 1 \) we can neglect the \( r^{2\epsilon} \) in the denominator, giving

\[
\theta \approx C \pm \frac{Br^\epsilon}{A \nu \epsilon}anumber{(3.122)}
\]

In this case the boundary spirals toward the singularity, but flattens out as it nears the singularity, only making a finite number of revolutions.
3.6.3 Behaviour for Special Boundary Conditions

Here we look at the behaviour near a singularity for those boundary conditions examined earlier in the chapter. Rather than derive all the results here, we present a table, Table 3.1, which summarises the possible behaviour. The behaviour near a line singularity, \( \eta = Ax^\nu \), and a radial singularity, \( \eta = Ar^\nu \), both depend upon the same parameters, \( \nu - \sigma - 1 \) and \( B \). These parameters are shown for various boundary conditions.

When \( \nu - 1 - \sigma < 0 \) we get (3.114) for the linear singularity and (3.122) for the radial singularity. When \( \nu - 1 - \sigma = 0 \) we get (3.111) for the linear singularity and (3.120) for the radial singularity. When \( \nu - 1 - \sigma > 0 \) we have no solution curves near the singularity.

Here we look at the behaviour near a singularity for those boundary conditions examined earlier in the chapter. Rather than derive all the results here, we present a table, Table 3.1, which summarises the possible behaviour. The behaviour near a line singularity, \( \eta = Ax^\nu \), and a radial singularity, \( \eta = Ar^\nu \), both depend upon the same parameters, \( \nu - \sigma - 1 \) and \( B \). These parameters are shown for various boundary conditions.

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<table>
<thead>
<tr>
<th>( \nabla \eta \cdot \hat{n} = )</th>
<th>( \nu ) Range</th>
<th>( \sigma )</th>
<th>( B )</th>
<th>( \nu - \sigma - 1 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( c )</td>
<td>all</td>
<td>0</td>
<td>( c )</td>
<td>( \nu - 1 )</td>
</tr>
<tr>
<td>( b\eta )</td>
<td>all</td>
<td>( \nu )</td>
<td>( Ab )</td>
<td>( -1 )</td>
</tr>
<tr>
<td>( b + c\eta )</td>
<td>( \nu &lt; 0 )</td>
<td>( \nu )</td>
<td>( cA )</td>
<td>( -1 )</td>
</tr>
<tr>
<td></td>
<td>( \nu = 0 )</td>
<td>0</td>
<td>( b + cA )</td>
<td>( -1 )</td>
</tr>
<tr>
<td></td>
<td>( \nu &gt; 0 )</td>
<td>0</td>
<td>( b )</td>
<td>( \nu - 1 )</td>
</tr>
<tr>
<td>( \cos \gamma \sqrt{1 + \nabla \eta^2} )</td>
<td>( \nu &gt; 1 )</td>
<td>0</td>
<td>( \cos \gamma )</td>
<td>( \nu - 1 &gt; 0 )</td>
</tr>
<tr>
<td></td>
<td>( \nu = 1 )</td>
<td>0</td>
<td>( \cos \gamma \sqrt{1 + A^2} )</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>( \nu &lt; 1 )</td>
<td>( \nu - 1 )</td>
<td>( \cos \gamma</td>
<td>A\nu</td>
</tr>
</tbody>
</table>

Table 3.1: The behaviour of boundary tracing near a singularity for a selection of boundary conditions

The use of this table can be seen in the following example.

**Example 9.** For a radial solution \( \eta = Ar^\nu \) with the constant contact condition \( \nabla \eta \cdot \hat{n} = \cos \gamma \sqrt{1 + \nabla \eta^2} \) we have the following cases. If

\( \nu > 1 \): In this case the table gives \( \nu - 1 - \sigma > 0 \), so there are no solutions locally.

Also, the solution does not have a singularity at \( y = 0 \).

\( \nu = 1 \): In this case the table gives \( \nu - 1 - \sigma = 0 \) and \( B = \cos \gamma \sqrt{1 + A^2} \), so we
get solutions when \( \left| \frac{B}{A^\nu} \right| < 1 \), i.e.

\[
\left| \frac{\cos \gamma \sqrt{1 + A^2}}{A} \right| < 1
\]  \hspace{1cm} (3.123)

which is true when \( |A| > \cot^2 \gamma \). The traced boundary is locally

\[
\theta = C \pm \frac{\cos \gamma \sqrt{1 + A^2}}{\sqrt{A^2 \sin^2 \gamma - \cos^2 \gamma}} \log(r)
\]  \hspace{1cm} (3.124)

and spirals around the singularity an infinite number of times.

\( \nu < 1 \): In this case \( \nu - 1 - \sigma = 0 \), and \( B = A\nu \cos \gamma \) so we get solutions when

\[
\left| \frac{A\nu \cos \gamma}{A^\nu} \right| < 1
\]  \hspace{1cm} (3.125)

which is always true (so long as \( \nu \neq 0 \)). In this case the boundary curves are locally

\[
\theta = C \pm \frac{A\nu \cos \gamma}{\sqrt{A^2 \nu^2 - A^2 \nu^2 \cos^2 \gamma}} \log(r) = \cot \gamma \log(r)
\]  \hspace{1cm} (3.126)

Again the traced boundaries spiral around the singularity an infinite number of times.

### 3.7 Conclusion

This chapter has introduced a consistent terminology for boundary tracing and derived many results for boundary tracing with general flux boundary conditions.

It was seen that the domain of a base function, \( \eta \), can be divided into regions where traced boundaries, satisfying a given boundary condition, can or cannot exist. These domains are called the viable and non-viable regions respectively. The boundary between these domains is called the terminal curve and in symmetric cases is often a suitable boundary.

Boundary geometry was determined, with relatively simple results for boundary direction and curvature.

The boundary tracing manifold, developed in this chapter, allows interpretation of the boundaries as smooth flows on a smooth manifold. As such it is a useful tool in understanding the behaviour of traced boundaries in a geometric manner.

Results for well-known boundary conditions and/or symmetrical geometry were also derived. These results are used frequently in the following chapters.
CHAPTER 4

Examples of Boundary Tracing

This chapter examines several examples of boundary tracing. These illustrate many of the results from Chapter 3 and display the wide variety of behaviour that can arise from boundary tracing.

The first section covers five simple examples (Examples 10 to 14) without reference to a governing PDE.

The two remaining sections demonstrate the use of boundary tracing to extract information in a PDE context. The PDEs considered are Poisson's equation and the constant mean curvature equation. These provide simple examples of the use of boundary tracing to obtain useful results for a PDE. Techniques similar to those used here will be used in the later chapters.

4.1 Some Simple Examples

In this section we illustrate boundary tracing using some simple base functions. The traced boundaries for these cases display a surprisingly rich and interesting variety of behaviours.

Examples 10 and 11 look at the solution for the radial function $\eta = (x^2+y^2)/2$, for constant flux and constant contact angle boundary conditions respectively. Analytic expressions for the boundary curve can be extracted for these cases. It is also shown that the terminal curve is an acceptable boundary and that the curvature formulae derived earlier give correct results.

In Example 12 we examine the behaviour for $\eta = xy$ with the boundary condition $\nabla \eta \cdot \hat{n} = c$. This example shows many of the features discussed in Chapter 3. In this case exact analytic descriptions are not available for all traced boundaries. Examination of the boundary curves on the associated manifold shows the existence of eight smooth curves tangential to the terminal curve at a saddle type critical terminal point. Four of these curves are straight lines, the other four are smooth curves. All other boundaries have cusps where they hit the terminal curve.

In the above examples the viable regions are unbounded. Example 13 is an example where the viable region is bounded. The boundaries are then traced numerically, and when viewed on the manifold exhibit singularities. Using topological arguments we show that for any case where the viable domain is bounded there must be a singularity of the direction field on the associated manifold. This example is also used to show that it is not always possible to piece together boundaries to give sensible domains.
Chapter 4. Examples of Boundary Tracing

The final example in this section examines the base function $\eta = \sin \rho x \sin \mu y$ with boundary condition $\nabla \eta \cdot \hat{n} = c$. This example shows that the viable domain can change substantially when parameters in the boundary condition are changed. In particular, the viable domain changes from a connected “mesh” into disjoint “islands”, which then disappear altogether. The resulting change in the topology of the associated manifold induces dramatic changes in the boundary behaviour.

**Example 10.** Here we look at the symmetric case $\eta = \frac{x^2 + y^2}{2}$ with the boundary condition $\nabla \eta \cdot \hat{n} = 1$. The terminal curves are given by $\nabla \eta^2 - 1 = 0$. In this case $\nabla \eta = [\frac{x}{y}]$ and the terminal curve is the unit circle. The feasible region is the region external to the unit disc, $x^2 + y^2 > 1$.

We know from Subsection 3.1.5 that near the terminal curve traced boundaries are parallel to the contours of $\eta$. Due to the radial symmetry of $\eta$ the terminal curve is the contour $\eta = 1/2$. Thus the boundaries touch the terminal curve tangentially.

According to Subsection 3.1.5, in this case the terminal curve satisfies the boundary condition. This is easily verified. On the terminal curve $\nabla \eta = \hat{n} = [\frac{x}{y}]$ and $\hat{n} = [\frac{y}{x}]$, thus $\nabla \eta \cdot \hat{n} = x^2 + y^2 = 1$ as required.

Due to the symmetry of $\eta$ the results of Subsection 3.5.4 can be used to obtain an expression for the traced boundaries. This gives

$$C \pm \theta = \int \frac{G \, dr}{r \sqrt{\eta^2 - G^2}}$$

$$= \int \frac{dr}{r \sqrt{r^2 - 1}}$$

$$= \sin^{-1} \frac{1}{r}$$

$$r \sin(C \pm \theta) = 1$$

$$x \sin(C) + y \cos(C) = 1$$

Thus the boundaries are simply straight lines tangential to the unit circle. Combining these boundaries and the $x^2 + y^2 = 1$ boundary we can construct a variety of domains including (but not limited to) polygonal, lenticular and teardrop shaped domains. The traced boundaries and an example domain can be seen in Figure 4.1.

Since the traced boundaries are straight lines we expect zero curvature everywhere in the interior of the viable domain. Through each point on the terminal curve there are two boundary curves; a line and the unit circle. Thus we must have two values for the curvature, 0 and 1. The curvature can be calculated using the results of Subsection 3.1.6.
4.1. Some Simple Examples

Figure 4.1: The straight line solution curves for $\nabla \eta \cdot \hat{n} = 1$, $\eta = (x^2 + y^2)/2$ (left), and a domain constructed from them (right).

The curvature away from the terminal curve is given by (3.28)

$$\kappa = \frac{\nabla F \cdot \dot{\hat{r}} - \hat{n}^T F \dot{\hat{r}}}{\nabla \eta \cdot \dot{\hat{r}}}$$

In the viable domain

$$\nabla F = 0 \quad H = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \hat{n} \cdot \dot{\hat{r}} = 0$$

Thus

$$\kappa = 0$$

in the interior of the viable domain.

The curvature of the traced boundaries at the terminal curve is given by (3.34)

$$\kappa^2 \nabla \eta \cdot \hat{n} + \kappa (\hat{n}^T H \hat{n} - 2 \hat{r}^T H \dot{\hat{r}} + \nabla F \cdot \hat{n}) + \dot{\hat{r}}^T H \dot{\hat{r}} - J(\dot{\hat{r}}, \dot{\hat{r}}, \hat{n}) = 0$$

On the terminal curve

$$\nabla \eta \cdot \hat{n} = 1 \quad \hat{n}^T H \hat{n} = 1 \quad \dot{\hat{r}}^T H \dot{\hat{r}} = 1$$

$$\nabla F = 0 \quad H^F = 0 \quad J = 0$$

so

$$\kappa^2 - \kappa = 0$$

Thus $\kappa = 1$ or $\kappa = 0$ on the terminal curve as expected.

The behaviour on the associated manifold can also be examined. In this case the manifold is given by $z^2 = x^2 + y^2$. The solution curves on this manifold can be seen in Figure 4.2. These curves are straight lines in three dimensions.
Figure 4.2: The curves derived from boundary tracing for $\eta = (x^2 + y^2)/2$ with boundary condition $\nabla \eta \cdot \hat{n} = 1$ projected onto the associated manifold $z^2 = x^2 + y^2$ are straight lines.

**Example 11.** Here we look at the same base function as Example 10 but with constant contact angle boundary conditions:

$$\nabla \eta \cdot \hat{n} = \cos \gamma \sqrt{1 + \|\nabla \eta\|^2}$$

(4.1)

In this case $F = G(r) = \cos \gamma \sqrt{1 + r^2}$, giving

$$\theta = C \pm \frac{\cos \gamma}{\sin \gamma} \int \frac{\sqrt{1 + r^2}}{r \sqrt{r^2 - \cot^2 \gamma}} \, dr$$

(4.2)

This can be integrated in terms of the Appell hypergeometric function, $F_1$. As in Example 10 the terminal curve, $r = \cot \gamma$, is another valid boundary.

The resulting curves can be seen in Figure 4.3, for $\gamma = \pi/4$. The traced boundary curves can be seen on the associated manifold in Figure 4.4.

New domains can be constructed by piecing together portions of the traced curves. Typical domains are shown in Figure 4.5.

**Example 12.** This example investigates the behaviour of traced $\nabla \eta \cdot \hat{n} = 1$ boundaries for $\eta = xy$. First we determine the valid region for solution curves and the terminal curves.

For this non-homogeneous Neumann boundary condition $\Phi = \|\nabla \eta\|^2 - 1 = x^2 + y^2 - 1$, so the terminal curve, $\Phi = 0$, is $x^2 + y^2 = 1$. Clearly $\Phi < 1$ for $x^2 + y^2 < 1$, so the viable domain is $x^2 + y^2 \geq 1$.

Although exact solutions for the traced boundaries cannot be obtained, a large amount of information about their behaviour can be derived analytically and they can be traced numerically.
4.1. Some Simple Examples

First we can look at the boundary directions. These are easily obtained by assuming \( \mathbf{n} = (n_x, n_y) \) and \( n_x^2 + n_y^2 = 1 \). Then the boundary condition \( \nabla \eta \cdot \mathbf{n} = x n_y + y n_x = 1 \). Solving these for \( n_x \) and \( n_y \) gives

\[
\begin{align*}
n_x &= \frac{y - x \sqrt{x^2 + y^2 - 1}}{x^2 + y^2} \\
n_y &= \frac{x + y \sqrt{x^2 + y^2 - 1}}{x^2 + y^2}
\end{align*}
\]

or

\[
\begin{align*}
n_x &= \frac{y + x \sqrt{x^2 + y^2 - 1}}{x^2 + y^2} \\
n_y &= \frac{x - y \sqrt{x^2 + y^2 - 1}}{x^2 + y^2}
\end{align*}
\]

This can be integrated numerically to give the boundary curves. Field plots for the two branches of the direction field and the numerically traced boundaries can be seen in Figure 4.6.

The critical terminal points where the traced boundary is tangential to the terminal curve occur where \( \nabla \eta \) and \( \nabla \Phi = H \nabla \eta \) are parallel. This gives

\[
\frac{\nabla \eta^T H \nabla \eta}{\| \nabla \eta \| \| H \nabla \eta \|} = 1
\]

\[
\frac{2xy}{x^2 + y^2} = \pm 1
\]

\[
(x \pm y)^2 = 0
\]

These points must also fall on the terminal curve \( x^2 + y^2 = 1 \), so there are 4 points where the traced boundaries will be tangential to the terminal curve. These are

\[
x = (\pm 1/\sqrt{2}, \pm 1/\sqrt{2})
\]
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Figure 4.4: Image showing the behaviour of boundaries with boundary condition \( \frac{\nabla \eta \cdot \hat{n}}{\sqrt{1 + (\nabla \eta)^2}} = \cos \gamma \) with \( \gamma = \pi/2 \) and \( \eta = (x^2 + y^2)/2 \) on the associated manifold.

From Figure 4.6 we can see that there are two curves through these special points, one of which is the straight line

\[
x \pm y = \pm \sqrt{2}
\]  

(4.5)

The other curve cannot be found analytically. Using the result for curvature at critical terminal points, (3.34), the curvatures at the point can be determined. Only the point \((1/\sqrt{2}, 1/\sqrt{2})\) need be considered, as by symmetry the curvatures at the other critical terminal points are the same. Here

\[
\eta = xy \\
\nabla \eta = \begin{bmatrix} y \\ x \end{bmatrix} \\
H = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \\
J = 0 \\
F = 1 \\
\nabla F = 0 \\
H^F = 0 \\
\hat{\tau} = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 \\ 1 \end{bmatrix} \\
\hat{n} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}
\]

The equation for the curvature, (3.34),

\[
\kappa^2(\nabla \eta \cdot \hat{n}) + \kappa(\hat{n}^T H \hat{n} - 2 \hat{T}^T H \hat{T} + \nabla F \cdot \hat{n}) + \hat{T}^T H^F \hat{T} - J(\hat{\tau}, \hat{\tau}, \hat{n}) = 0
\]

becomes

\[
\kappa^2 + 3\kappa = 0
\]  

(4.6)

This gives the curvature \( \kappa = 0 \), for the straight line and \( |\kappa| = 3 \), for the other curve.
Figure 4.5: A variety of domains constructed from the traced boundaries of $\eta = (x^2 + y^2)/2$ with the boundary condition $\frac{\nabla \eta \cdot \hat{n}}{\sqrt{1 + (\nabla \eta)^2}} = \cos \gamma$.

We can also examine the behaviour of the curves on the associated manifold $z^2 = x^2 + y^2$. As can be seen in Figure 4.7 these curves are not as simple as the curves in earlier examples. This is not surprising as the traced boundaries can exhibit a far wider range of behaviours than they did for the symmetric cases. The figure shows that there are boundaries that switch from the upper half of the manifold to the lower half of the manifold and these transitions cause the cusps that can be seen in the two-dimensional image, Figure 4.6. It can also be seen that there are saddle points at the critical terminal points on the manifold. The separatrices of the saddle points form the two curves examined earlier.

Although we have found many boundaries with $\nabla \eta \cdot \hat{n} = 1$ it is impossible to piece them together to create a bounded domain with $\nabla \eta \cdot \hat{n} = 1$ along its boundary. The problem is with the orientation of the boundaries, shown in Figure 4.8. It can be seen that no closed curves can be constructed from the traced boundaries while maintaining their orientation. This is made evident by breaking the domain into pieces. For example two pieces would be AIH and BKJIA in Figure 4.8. It is clear from the directions shown in the figure that traced boundaries cannot move from AIH into BKJIA. By looking at the more complete breakup of the domain shown in Figure 4.9, showing the possible paths for traced curves, we find that the graph is acyclic, consequently
Chapter 4. Examples of Boundary Tracing

Figure 4.6: The two branches of the direction field and the traced boundaries when \( \eta = xy \) with boundary condition \( \nabla \eta \cdot \hat{n} = 1 \). (Note the unit circle is not a boundary)

Figure 4.7: The traced boundaries projected onto the associated manifold for \( \eta = xy \) with the boundary condition \( \nabla \eta \cdot \hat{n} = 1 \).

any closed domain must fall entirely within one of the pieces. It is easy to see that none of the pieces can contain a closed boundary. For example in AIH both branches of the traced boundary have \( \hat{\tau} \cdot \hat{i} < 0 \) thus can contain no closed boundary. Since there can be no closed traced boundaries that switch between pieces and no piece can contain a closed boundary, there must be no closed boundaries with \( \nabla \eta \cdot \hat{n} = 1 \) for \( \eta = xy \).

The non-existence of closed domains is not surprising when we recognise that \( \eta = xy \) satisfies \( \nabla^2 \eta = 0 \) and thus around any closed curve we have

\[
\oint_C \nabla \eta \cdot \hat{n} \, ds = 0
\]

Consequently no closed curves with \( \nabla \eta \cdot \hat{n} = 1 \) can exist.
We can construct valid domains if we are willing to accept infinite domains, or domains with $\nabla \eta \cdot \hat{n} = \pm 1$. Examples of these can be seen in Figure 4.10 and Figure 4.11.

**Example 13.** In the previous examples the viable domains have been unbounded. In this example we construct a solution where the traced boundaries are restricted to a bounded domain for the boundary condition $\nabla \eta \cdot \hat{n} = \beta$. To achieve this we need a function which has sufficiently large, but continuous and bounded, gradient over a limited area.

A simple one dimensional function with this property is $\arctan(x)$. From this we can obtain an appropriate two dimensional function

$$\eta = \arctan(x) + \arctan(y) \quad (4.7)$$

A three dimensional plot showing the large gradient near the origin can be seen in Figure 4.12. The gradient is

$$\nabla \eta = \begin{bmatrix} \frac{1}{1+x^2} \\ \frac{1}{1+y^2} \end{bmatrix} \quad (4.8)$$

This gives

$$\|\nabla \eta\| = \sqrt{\frac{1}{(1+x^2)^2} + \frac{1}{(1+y^2)^2}} \quad (4.9)$$

A vector field plot of $\nabla \eta$ with contours of $\|\nabla \eta\|$ can be seen in Figure 4.13.
Figure 4.9: The possible directions of flow for the traced boundaries (using the domains from Figure 4.8) can be seen to be acyclic.

Figure 4.10: An unbounded domain with boundary condition $\nabla \eta \cdot \hat{n} = 1$ and solution $\eta = xy$.

Near the origin $||\nabla \eta|| \approx \sqrt{2}$ and the contours of $||\nabla \eta||$ form closed curves. It can be shown that the curves $||\nabla \eta|| = \beta$, for $1 < \beta < \sqrt{2}$, are closed\(^1\). Thus

\(^1\)Assuming $\beta > 1$, then due to symmetry we can assume without loss of generality that $0 \leq x \leq y$, then

$$||\nabla \eta||^2 = \frac{1}{(1 + x^2)^2} + \frac{1}{(1 + y^2)^2}$$  \hspace{1cm} (4.10)

$$\leq 1 + \frac{1}{(1 + y^2)^2}$$  \hspace{1cm} (4.11)

So

$$\nabla \eta^2 - \beta^2 \leq (1 - \beta^2) + \frac{1}{(1 + y^2)^2}$$  \hspace{1cm} (4.12)

Thus for $y$ large $y \nabla \eta^2 - \beta^2 < 0$ and consequently the viable domain is bounded.
4.1. Some Simple Examples

Figure 4.11: A variety of finite domains with solution $\eta = xy$, having boundary condition $\nabla \eta \cdot \hat{n} = 1$ on solid boundaries and $\nabla \eta \cdot \hat{n} = -1$ on dotted boundaries.

Figure 4.12: The function $\eta = \arctan(x) + \arctan(y)$ shown in three dimensions.

taking the boundary condition to be $\nabla \eta \cdot \hat{n} = \beta$, with $1 < \beta < \sqrt{2}$, creates a bounded viable domain, as viable domain is given by $\nabla \eta^2 - \beta^2 > 0$.

Looking at the case $\beta = 1.2$ we can find two direction fields for the boundary direction. (Algebraic calculations performed in Mathematica are omitted here for brevity.) These fields can be integrated numerically to give the boundaries. The two branches for the boundary direction and the traced boundaries are shown in Figure 4.14.

Now recall from Section 3.3 that the two direction fields can be considered to be one direction field on a manifold $M$. In this case the manifold is topologically equivalent to a sphere.

A well-known theorem (the hairy ball theorem) is

**Theorem 1.** A sphere of local dimension $n$, $S^n$ has nowhere vanishing (differentiable) vector field if and only if $n$ is odd

Conversely if $\beta \leq 1$ then at the point $(0, t)$, $\nabla \eta^2 = 1+(1+t^2)^{-2}$, so $\nabla \eta^2 - \beta^2 = 1-\beta^2+(1+t^2)^{-2} > 0$ so $(0, t)$ is in the viable domain and the viable domain in unbounded.
Figure 4.13: This figure shows $\nabla \eta$ for $\eta = \arctan(x) + \arctan(y)$. The smooth curves are contours of $||\nabla \eta||$.

Figure 4.14: Boundary tracing for $\eta = \arctan(x) + \arctan(y)$, with $\nabla \eta \cdot \hat{n} = 1.2$. Left and Center: The two direction fields. Right: The traced boundaries.

A derivation of this result can be found in Greenberg [12] as Theorem 16.5.

Since $M$ is topologically equivalent to a sphere, $S^2$, there must be a singularity or zero vector in the direction field by Theorem 1. As the direction field on the manifold consists of unit vectors there can be no zero. Thus there must be a singularity. However, the singularity cannot occur on either the top or the bottom halves of the ball, since the vector field is differentiable there. The singularity must occur on the equator of the ball. We find that the two singularities for this example are spiral type critical terminal points on the manifold. These can be seen in Figure 4.15.

The domain with traced boundaries is topologically equivalent to a square with two sets of boundaries, both running toward the top of the square, as shown in Figure 4.16. From this figure it is evident that no closed curve can be
4.1. Some Simple Examples

Figure 4.15: The traced boundaries where the viable domain is topologically equivalent to a ball must have singularities, in this case spiral singularities.

formed using the traced boundaries while maintaining the correct orientation. Typical boundaries can be seen in Figure 4.17.

While none of these boundaries are physically acceptable, sensible domains with a combination of the boundary conditions \( \nabla \eta \cdot \hat{n} = \pm \beta \) can be constructed.

Figure 4.16: The traced boundaries in the compact domain are topologically equivalent to these curves on a square, showing that there can be no closed loops.

Example 14. \( \sin \rho x \sin \mu y \) solves Helmholtz's equation \( (\nabla^2 + k^2)\eta = 0 \) in \( (0, \pi/\rho) \times (0, \pi/\mu) \) with \( \eta = 0 \) on the boundary when \( k^2 = \rho^2 + \mu^2 \).
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Figure 4.17: Typical traced boundaries with interior/exterior indicated for $\nabla \eta \cdot \hat{n} = c$ and $\eta = \arctan(x) + \arctan(y)$.

It is easy to see that the lines $x = (2N + 1)\pi/(2\rho)$ and $y = (2N + 1)\pi/(2\mu)$ all satisfy $\nabla \eta \cdot \hat{n} = 0$ for any integer $N$.

There are also other solutions. For example the boundaries

$$y = \frac{1}{\mu} \arccos(C \cos(\rho x^2)\mu^2)^{\rho^{-2}}$$

also satisfy the homogeneous Neumann conditions. These curves (for $\mu = 1$, $\rho = 1$) can be seen in Figure 4.18.

For the boundary condition $\nabla \eta \cdot \hat{n} = c$, the viable domain changes shape drastically depending upon the choice of $c$. In particular for $c = 0$ the entire plane is viable, for $0 < c < c_1 = \frac{\rho \mu}{\sqrt{\rho^2 + \mu^2}}$ the plane is punctured by regularly spaced holes. For $c_1 < c < c_{MAX} = \max(\{|\rho|, |\mu|\})$ the viable domain consists of isolated islands and for $c > c_{MAX}$ there is no viable domain.

When $c = c_1$ the domain is split into a checker-board of rectangles, alternating between the viable domain and non-viable domains. The lines of the checker-board are given by

$$x = \pm \frac{1}{\rho} \cos^{-1} \left( \frac{\pm \mu}{\sqrt{\mu^2 + \rho^2}} \right)$$

(4.13)
4.1. Some Simple Examples

Figure 4.18: Curves with $\nabla \eta \cdot \hat{n} = 0$ for $\eta = \sin x \sin y$.

and

$$y = \pm \frac{1}{\mu} \cos^{-1} \left( \pm \frac{1}{\sqrt{\mu^2 + \rho^2}} \right)$$

(4.14)

$$y = \pm \frac{1}{\mu} \cos^{-1} \left( \pm \frac{1}{\sqrt{\mu^2 + \rho^2}} \right)$$

(4.15)

Since the maximum of $\|\nabla \eta\|$ is $c_{MAX}$, for $c \geq c_{MAX}$ there is no viable domain. Thus as $c$ approaches $c_{MAX}$ the islands shrink further, until they finally disappear.

Although the boundaries cannot be calculated exactly, they can be calculated numerically. An image for $c_1 < c < c_{MAX}$ with the boundaries traced on the manifold can be seen in Figure 4.19 (See Figure C.3 for colour version). Note that the boundaries wrap around like a ball of string. A similar image for $0 < c < c_1$ can be seen in Figure 4.20 (See Figure C.4 for colour version).

In the cases where the viable domains form isolated islands the situation is similar to that in Example 13, and we are unable to construct sensible boundaries. However the case where the viable domain is connected warrants closer attention. Only the simpler case where $\mu = \rho$ will be considered further. In this case some of the traced boundaries are straight lines, as can be seen in Figure 4.20.

First we must examine the direction of the boundary curves. Better understanding of the directions can be obtained from Figure 4.21. Here we have assumed an orientation for the curve AB. From this we can deduce the orientation of CD. Since CD ends on the terminal curve at D we can also deduce
Chapter 4. Examples of Boundary Tracing

Figure 4.19: The traced boundaries, shown in two dimensions and on the associated manifold, for $\eta = \sin px \sin \mu y$ with the boundary condition $\nabla \eta \cdot \hat{n} = c$ with $c_1 < c < c_{MAX}$, form balls. (See Figure C.3 for colour version)

the direction of $DE$. These curves then give the directions of the lines $af$, $be$, $ch$ and $dg$.

In a similar manner we can obtain directions for all the straight lines. These form a checkerboard type pattern, shown in Figure 4.22. Here it can be seen that boundaries like the square ABCDA do not form valid boundaries, but the square abcd does. It is also evident that we can construct rectangular domains such as felkf. Examples of other domains that can be obtained (rotated by $\pi/4$) are shown in Figure 4.23. These domains are not only sensible but potentially useful. The geometry of the domains does not suggest that they admit exact solutions to Helmholtz's equation. It is not clear how one could construct solutions (especially exact) in such domains.

Since there are other traced boundaries near the straight line boundaries it is possible to modify the domains shown in Figure 4.23. For example Figure 4.24 shows a trivial modification that can be done to a simple square domain.

Note: Any boundary defining an interior domain also defines an exterior domain after translation, and vice versa. This is equivalent to multiplying $\eta$ by $-1$.

The purpose of the above examples was to establish the variety of traced boundary behaviours rather than display practical applications. In the following sections boundary curves linked to PDEs will be examined.

4.2 Poisson's Equation
4.2. Poisson’s Equation

4.2.1 Introduction Poisson’s equation

\[ \nabla^2 \eta = K \]  \hspace{1cm} (4.16)

arises in steady state heat conduction and field problems.

Due to the simplicity of its radially and translationally symmetric solutions, Poisson’s equation serves as a simple introduction to the techniques of boundary tracing.

When the boundary condition is

\[ \nabla \eta \cdot \hat{n} = c \]  \hspace{1cm} (4.17)

there is either an infinite number of solutions in a domain (differing only by an additive constant) or no solutions in the domain. Using the divergence theorem we can see that there will only be solutions when

\[ \frac{K |\Omega|}{c |\partial \Omega|} = 1 \]  \hspace{1cm} (4.18)

For the steady state heat conduction problem this requirement is conservation of energy; heat generated in the interior of the domain must be balanced by the heat leaving through the boundary. In general \( K \) or \( c \) are chosen so that this is satisfied.

If \( \eta \) is a solution to the Poisson’s equation and \( \mu \) is a solution to Laplace’s equation, \( \nabla^2 \mu = 0 \), then \( \eta + \lambda \mu \) is also a solution to the Poisson’s problem for any \( \lambda \in \mathbb{R} \).
Chapter 4. Examples of Boundary Tracing

Figure 4.21: The directions for selected traced boundaries for $\eta = \sin \rho x \sin \rho y$ when the viable domain is connected. (The nonviable domains are shown in grey.)

Figure 4.22: The directions of the straight line boundaries for $\eta = \sin \rho x \sin \rho y$, $\nabla \eta \cdot \mathbf{n} = c$.

In Section 2.2 it was mentioned that boundary tracing had previously been used with Poisson's equation in the determination of cooling times for "pseudo-ellipses" by McNabb et al. [22]. The boundary conditions used were homogeneous Robin boundary conditions

$$ a \nabla \eta \cdot \mathbf{n} + b \eta = 0 \quad (4.19) $$

and similar boundary conditions will be considered here in Section 4.2.6.

The constant flux boundary conditions, $\nabla \eta \cdot \mathbf{n} = c$, will be considered first, followed by Robin boundary conditions.
4.2. Poisson’s Equation

Figure 4.23: Example domains that can be constructed using the straight line boundaries for $\eta = \sin \rho x \sin \rho y$.

Figure 4.24: A modified square boundary for $\eta = \sin \rho x \sin \rho y$ with $\nabla \eta \cdot \hat{n} = c$.

4.2.2 Simple Solutions The Poisson’s equation admits a variety of simple exact solutions. We will not attempt to survey the known solutions here, restricting our attention to the simpler solutions. The simplest non-trivial solutions are quadratic functions. In particular

$$\eta = x^T M x + b \cdot x + d$$  \hspace{1cm} (4.20)

is a solution to Poisson’s equation if $Tr(M) = \frac{K}{2}$. These solutions include

One Dimensional Solutions

$$\eta = \frac{K}{2} y^2 + C_1 y + C_2$$  \hspace{1cm} (4.21)

Radial Solutions

A polynomial radial solution is given by

$$\eta = \frac{Kr^2}{4} + C_1.$$  \hspace{1cm} (4.22)
The general radial solution can be obtained by adding the radial solution to Laplace’s equation

\[ \eta = \frac{Kr^2}{4} + C_1 + C_2 \log(r) \]  

(4.23)

4.2.3 Channel Solution Here we consider the one dimensional solution

\[ \eta = \frac{K}{2} y^2 + C \]  

(4.24)

which is the solution to Poisson’s equation with boundary condition

\[ \nabla \eta \cdot \hat{n} = c \]  

(4.25)

on the lines \( y = \pm \frac{c}{K} \).

It will be shown that there are other boundaries satisfying the boundary condition (4.25) which give the same solution.

4.2.4 Boundary Tracing The terminal curves for this boundary condition are \( \| \nabla \eta \| = c \), giving \( y = \pm \frac{c}{K} \), which are also valid boundary curves. As was mentioned in Subsection 3.1.5 it is not unusual for the terminal curves and the boundary curves to coincide for symmetric \( \eta \).

From the position of the terminal curves we find the viable regions for boundary tracing to be \( |y| \geq \left| \frac{c}{K} \right| \). These regions can be seen in Figure 4.25.

Figure 4.25: This figure shows the breakup of the domain of \( \eta = \frac{K}{2} y^2 \) into several pieces. The sections denoted A are the viable domains \( |y| \geq \left| \frac{c}{K} \right| \). The region marked B is the non-viable region. The lines \( y = \pm \frac{c}{K} \), marked C, are the terminal curves.
4.2. Poisson's Equation

Since \( \eta \) is of the form \( \eta = f(y) \) we can use the results of Subsection 3.5.1. That is the boundary curves are given by

\[
c \int \frac{dy}{\sqrt{\eta_y^2 - c^2}} = x + \delta
\]

This gives

\[
c \int \frac{dy}{\sqrt{K^2y^2 - c^2}} = x + \delta
\]

This integral can be solved and inverted to get \( y(x) \), giving

\[
y = \pm \frac{c}{K} \cosh \left( \frac{K}{c}(x + \delta) \right)
\]

where \( \delta \) is an arbitrary constant. The constant \( \delta \) represents arbitrary translation of the solution curve in the \( x \) direction. The curves are tangential to the \( y = \pm \frac{c}{K} \) boundary/terminal curve at the point \( x = \delta \), and are symmetric about this point. The curve is shown in Figure 4.26.

![Figure 4.26: The traced boundary \( y = \frac{c}{K} \cosh \left( \frac{K}{c}(x + \delta) \right) \)](image)

It is easily verified that the curve given by (4.26) is a solution. The normal to the curve is

\[
\hat{n} = \frac{1}{\sqrt{1 + \sinh^2 \left( \frac{K}{c}(x + \delta) \right)}} \begin{bmatrix}
-\sinh \left( \frac{K}{c}(x + \delta) \right) \\
1
\end{bmatrix}
\]

\[
= \begin{bmatrix}
-\tanh \left( \frac{K}{c}(x + \delta) \right) \\
1 / \cosh \left( \frac{K}{c}(x + \delta) \right)
\end{bmatrix}
\]
Also

\[ \nabla \eta = \begin{bmatrix} 0 \\ Ky \end{bmatrix} = \begin{bmatrix} 0 \\ c \cosh\left(\frac{K}{c}(x + \delta)\right) \end{bmatrix} \]

so

\[ \nabla \eta \cdot \hat{n} = c \]

and the boundary satisfies the required boundary conditions.

Curvature The curvature of a curve in the plane is

\[ \kappa = \frac{|y''(x)|}{\left(1 + y'(x)^2\right)^{3/2}} \quad (4.27) \]

which for the boundary (4.26) gives (after some rearranging)

\[ |\kappa| = \frac{c}{Ky^2} \quad (4.28) \]

Similarly the curvature equations given in Chapter 3 for \( \eta = \eta(y) \), (3.91), give

\[ \kappa = \frac{F'(y)\eta_y - F(y)\eta_{yy}}{\eta_y^2} \]

\[ = \frac{-c\eta_y y}{\eta_y^2} \]

\[ = \frac{-c}{Ky^2} \]

where \( \nabla \eta \cdot \hat{n} = F(y) = c \). Thus the curvature derived using the technique from Chapter 3 matches the curvature derived from the curve using standard methods.

New Domains The curve derived by boundary tracing does not define a sensible domain for the Poisson's equation, as along the boundary \( \eta \to \infty \) as \( y \to -\infty \) which normally is not acceptable for physical reasons.

Several properties of the traced curve allow us to construct domains in which the solution is sensible. In particular a copy of the curve translated in the \( x \) direction will still satisfy \( \nabla \eta \cdot \hat{n} = 1 \). Several of these curves and the curve \( y = c/K \) can be combined in a piecewise manner to obtain new domains which still satisfy the boundary condition.

A simple example of the domains that can be constructed in this manner are shown in Figure 4.27. Light curves are the extension of the \( \cosh \) pieces and the dark
curves are the constructed boundary. A piecewise definition of the lower curve is:

\[
y = \begin{cases} 
\frac{c}{K} & \text{for } x < -W \\
\frac{c}{K} \cosh \left( \frac{K}{c} (x + W) \right) & \text{for } -W < x < 0 \\
\frac{c}{K} \cosh \left( \frac{K}{c} (x - W) \right) & \text{for } 0 < x < W \\
\frac{c}{K} & \text{for } x > W
\end{cases}
\]  

(4.29) 

for some \( W \). The upper curve can be described in a similar manner.

Figure 4.27: Two boundaries constructed by piecing together the \( \pm \cosh(x + C) \) traced boundaries for Poisson’s equation in a channel with \( K = 1 \) and \( c = 1 \).

In these new domains the solution is bounded and well behaved. Thus we have an exact solution to Poisson’s equation in a channel with spikes. There is some flexibility in the construction of these “spikes”, we can fix their height or width, but not both simultaneously. Domains having an arbitrary number of spikes on each boundary can be generated, resulting in a large and flexible family of domains.

Physically these results show that we can reshape a domain in certain ways without changing any of the global solution behaviour. Consequently if we measure the solution behaviour locally we cannot determine the boundary location, only regions where the boundary must lie (viable domains). In other words the inverse problem does not have unique solution.

A family of simple domains with sharp corners having known exact solution to Poisson’s equation have been generated. This is not so important for Poisson’s equation as there are many other solutions in simple domains. Similar techniques
will lead to new domains for the Laplace–Young equation, which is important as previously there were no known exact solutions in domains with corners.

4.2.5 Radial Tracing Boundary tracing simple radial solutions to the Poisson's equation gives interesting results; namely solutions in special polygonal domains including all triangles.

Recall that the radially symmetric solution to Poisson's equation is

$$\eta = \frac{K}{4}r^2 + A\ln r + B$$ (4.30)

Polynomial Case

First we consider the radial solutions to the Poisson problem which are bounded at the origin. These are

$$\eta = \frac{K}{4}r^2 + B$$ (4.31)

This has been investigated in Example 10 for $K = 2$, $B = 0$ and $\nabla \eta \cdot \hat{n} = 1$. Exactly the same method can be used to obtain straight line boundaries for this case.

The radially symmetric boundary satisfying the boundary condition is the circle $r = \frac{2\phi}{K}$, which is also the terminal curve. Thus we only expect boundaries satisfying the boundary conditions in the region $r \geq \left|\frac{2\phi}{K}\right|$. Using the same procedure as in Example 10 we obtain

$$r = \frac{2c}{K \cos(\pm \theta + \phi)}$$ (4.32)

which is the equation of straight lines tangential to the circle $r = \frac{2\phi}{K}$. Thus (4.31) is also the solution within polygonal domains with all sides (or their extensions) tangential to the circle $r = \frac{2\phi}{K}$. Two examples are the square with side length $4c/K$ and the equilateral triangle with side length $4\sqrt{3}c/K$ (which can be seen in Figure 4.28 (See Figure C.5 for colour version).

We can also find the solution in any triangle. The procedure is as follows. Find the in-circle of the triangle. This circle has radius $r_i$ and center $(x_i, y_i)$. Then the solution in the triangle is given by $\eta = \frac{K}{4}((x - x_i)^2 + (y - y_i))^2$. Additionally $K$ and $\phi$ must satisfy $Kr_i = 2c$.

Aside: Using the divergence result (4.18) on the radial solution in any polygon with all sides tangential to a circle we obtain the following geometrical theorem.

**Theorem 2.** Given a polygon with all sides (or their extensions) tangential to a circle of radius $R$, the ratio of the perimeter, $P$, to the area, $A$, is $A/P = R/2$. This is also the same ratio for the inscribed circle.
4.2. Poisson's Equation

Figure 4.28: The solution inside an equilateral triangle for the Poisson's equation. Left: Top view showing the terminal circle \( r = \frac{2c}{K} \) and the triangular domain. Right: Three dimensional figure showing the solution, viable (dark) and nonviable domains (light). (See Figure C.5 for colour version)

Proof. The polygon satisfies Poisson's equation with \( \nabla \eta \cdot \hat{n} = KR/2 \) on the boundary with \( \eta = \frac{K}{4} r^2 \). The condition \( \frac{K|\Omega|}{2|\partial \Omega|} = 1 \) gives

\[
\frac{|\Omega|}{|\partial \Omega|} = \frac{R}{2}
\]

The result extends trivially to Poisson's equation in three dimensions, where \( \eta = \frac{r^2 K}{6} \), and the boundaries are the planes \( n_1 x + n_2 y + n_3 z = 2c/K \) such that \( n_1^2 + n_2^2 + n_3^2 = 1 \). Higher dimensional extensions are also easily obtained. In a similar manner exact solutions to Poisson’s equation inside any \( n \)-dimensional polytope with all sides tangential to a \( n \)-sphere can be obtained. In particular we have the solution inside any platonic solid.

Similarly, the extension of Theorem 2 to higher dimensions holds:

**Theorem 3.** Given a \( N \)-dimensional polytope with all “edges” tangential to a given \( N \)-sphere, then the ratio of the \( N \)-volume, \( V_N \), to the \( N \)-surface area, \( S_N \), is the same for the sphere and the polytope, that is

\[
\frac{V_N}{S_N} = \frac{r}{N}
\]

Proof. As for Theorem 2.

**Full Case** We now consider the case where \( \eta \) includes the log term

\[
\eta = \frac{Kr^2}{4} + C_1 + A \log(r)
\]
While the the traced boundaries can be shown to be

\[
\theta = \frac{2}{c - \sqrt{c^2 - 2AK}} \mathcal{F} \left( \arcsin \left( \frac{-c + \sqrt{c^2 - 2AK}}{2A} r \right) | 2 \frac{c^2 - AK + c\sqrt{c^2 - 2AK}}{(c - \sqrt{c^2 - 2AK})^2} \right)
\]

(4.33)

this does not provide much useful information and only works for \( c^2 - 2AK > 0 \). Other, more useful, information can be derived by examining the geometry.

The terminal curves will again be radially symmetric. They are given by

\[
||\nabla \eta|| = \frac{K r^2 + 2A}{2r} = \pm c
\]

(4.34)

This has real solutions for \( r \) when \( c^2 > 2KA \). For this situation the solution is given by the positive values of

\[
r = \pm \frac{c \pm \sqrt{c^2 - 2KA}}{K}
\]

(4.35)

The values of \( r \) as a function of \( A \) are shown in Figure 4.29.

Figure 4.29: The radii of the terminal curves of \( \eta = \frac{K r^2}{4} + C_1 + A \log(r) \) with boundary condition \( \nabla \eta \cdot \hat{n} = c \) as a function of \( A \).

Defining \( A^* = c^2/(2K) \) we have five geometrically different cases depending on \( A \): \( A < 0, A = 0, 0 < A < A^*, A = A^* \) and \( A > A^* \).

In the cases \( A < 0 \) and \( 0 < A < A^* \) there is an inner viable region and an outer viable region. The \( A = 0 \) case is the polynomial case examined earlier (which had no inner viable domain). As \( A \) approaches 0 from either side the inner viable region shrinks to nothing.

It can be seen from Figure 4.29 that as \( A \) approaches \( A^* \) from below the gap between two viable domains becomes smaller until the domains merge. For \( A > A^* \) the viable domain is the entire plane.

The behaviour in each of the five cases has been calculated numerically and is shown in Figure 4.30. Domains constructed from the traced boundaries can be seen in Figure 4.31.
4.2. Poisson’s Equation

Figure 4.30: The five possible geometries for traced boundaries of $\eta = K r^2 / 4 + A \log r$ with $\nabla \eta \cdot \hat{n} = c$.

Figure 4.31: Domains constructed from the traced boundaries of $\eta = K r^2 / 4 + A \log r$ with $\nabla \eta \cdot \hat{n} = c$.

From Figure 4.30 we can see that the nature of the possible domains changes quite dramatically with the choice of $A$. For $A < 0$ domains can have holes in the interior. As $A \to 0$ the size of these holes reduces, until they disappear altogether. Also the other edges for $A < 0$ are quite curved, permitting the construction of domains like a square with slightly indented sides. As $A \to 0$ these sides straighten up, and for $A > 0$ the domain becomes a square with blown out sides. These changes and others can be seen in the example domains of Figure 4.31.

4.2.6 Robin Boundary Conditions In light of the previous work done with Robin boundary conditions and Poisson’s equation [22, 21] we will look briefly at the difficulties that arise, even for the relatively simple cases.

It is interesting that the homogeneous boundary conditions $\nabla \eta \cdot \hat{n} + \alpha \eta = 0$ are no easier to solve in the general case than the non-homogeneous $\nabla \eta \cdot \hat{n} + \alpha \eta = \beta$ boundary conditions.

Channel Solution Here the solution is

$$\eta = \frac{K}{2} y^2 + A$$
Chapter 4. Examples of Boundary Tracing

The boundary condition becomes

\[ \nabla \eta \cdot \hat{n} = \beta - \alpha \eta \]
\[ = (\beta - \alpha A) - \frac{K\alpha}{2} y^2 \]  
(4.36)

Using the results from Subsection 3.5.1 we obtain

\[ x = C \pm \int \frac{(\beta - \alpha A) - K\alpha y^2/2}{\sqrt{k^2 y^2 - ((\beta - \alpha A) - K\alpha/2y^2)^2}} \, dy \]  
(4.37)

This integral can be evaluated in terms of elliptic functions but is not exactly invertible to find \( y(x) \). A better understanding of the boundary behaviour can be obtained by examining the situation geometrically.

First we look for the terminal curves and viable domain. The viable domain is where \( \nabla \eta^2 - F^2 \geq 0 \). That is

\[ \Phi(y) = K^2 y^2 - \left( (\beta - \alpha A) - \frac{\alpha K}{2} y^2 \right)^2 \geq 0 \]  
(4.38)

Thus we have up to four terminal curves, given by

\[ y = \frac{\pm 1}{\alpha} \left( 1 \pm \sqrt{1 + \frac{2\alpha(\beta - \alpha A)}{K}} \right) \]  
(4.39)

which has real solutions for \( \alpha(\beta - \alpha A) \geq -1/2 \).

For the case where \( \alpha(\beta - \alpha A) < -1/2 \) there are no terminal curves, so the entire plane is either entirely viable or non-viable. We can determine which by looking at the origin. At the origin (4.38) becomes

\[ \Phi(0) = - (\beta - A\alpha)^2 \leq 0 \]  
(4.40)

so the origin can never be in the viable domain. Thus for the case when there are no terminal curves, there is no viable domain. In this case there are no solutions satisfying the required boundary conditions\(^2\). Similarly if \( \alpha(\beta - \alpha A) = -1/2 \) there is no viable domain.

Now if \( \delta = 2\alpha(\beta - \alpha A) > -1 \) the four terminal curves are the lines

\[ y = \frac{\pm 1}{\alpha} \left( 1 \pm \sqrt{1 + \delta} \right) \]  
(4.41)

These lines are \( \sqrt{1 + \delta}/\alpha \) on either side of the lines \( y = \pm 1/\alpha \).

\(^2\)of course this means that there was no channel with the prescribed boundary conditions to start with and the integral derived earlier will be imaginary.
4.2. Poisson’s Equation

We can easily see that the curves \( y = -(1 \pm \sqrt{1 + \delta})/\alpha \) satisfy the boundary condition with \( \hat{n} = \hat{i} \) and the curves \( y = (1 \pm \sqrt{1 + \delta})/\alpha \) satisfy it with \( \hat{n} = -\hat{i} \). This means the terminal curves are admissible boundaries.

There are six different geometries depending on the size of \( \delta \) and the sign of \( \alpha \). The three geometries with \( \alpha > 0 \) are shown in Figure 4.32, the three with \( \alpha < 0 \) are the same with the normals reversed.

![Figure 4.32: The three geometries for terminal curve boundaries for \( \eta = Ky^2/2 + A \) and \( \nabla \eta \cdot \hat{n} = \beta - \alpha \eta \) with \( \alpha > 0 \). The thick black lines are the terminal curves, with the shaded region on the opposite side to the normal. The grey regions are the viable region. Dashed lines are \( y = 0 \) and dotted lines \( y = \pm 1/\alpha \).](image)

More details can be obtained by examining \( \sin \theta \), where \( \theta \) is the angle between \( \nabla \eta \) and the tangent to the traced boundary.

\[
\sin \theta = \frac{\beta - \alpha \eta}{\| \nabla \eta \|} = \frac{\beta - \alpha A}{|Ky|} - \frac{\alpha \text{sgn}(K)}{2} \frac{1}{|y|}
\]  

(4.42)

There are three cases for the behaviour, these are shown in Figure 4.33.

In the case where \( \delta = 1 \), equation (4.37) can be integrated to give the boundaries exactly. The boundaries are circles with center on the \( y = 0 \) line and with radius \( 1/\alpha \).

In the other cases we can construct a variety of boundaries, as shown in Figure 4.34. Additionally channels with a change in width, or a slight bend, can be constructed in the \(-1 < \delta < 0\) case. Also for the \( \delta > 0 \) case solutions interior/exterior to infinite fingers or lenses can be constructed, these are shown in Figure 4.35.
4.3 Surfaces of Constant Mean Curvature

4.3.1 Introduction Surfaces of constant mean curvature (or CMC surfaces) show up in many contexts: gas dynamics, soap bubbles [7] and micro-gravity capillarity [8] providing a few examples.

The equation for surfaces of constant mean curvature is

$$\nabla \cdot \frac{\nabla \eta}{\sqrt{1 + |\nabla \eta|^2}} = \kappa$$  \hspace{1cm} (4.43)

This is the Laplace–Young equation in the absence of gravity and has received a great deal of attention from researchers in the area of surface tension, both theoretically and experimentally. A survey of recent work can be found in an article by Finn [10]. The special case $\kappa = 0$ is referred to as the minimal surface equation and is of importance in optimisation.
4.3. Surfaces of Constant Mean Curvature

Figure 4.35: Schematic of other Robin boundaries that can be traced from the solution to Poisson’s equation in a channel.

The boundary condition used in this chapter,

$$\frac{\nabla \eta}{\sqrt{1 + |\nabla \eta|^2}} \cdot \hat{n} = \cos \gamma \quad (4.44)$$

is the constant contact angle condition and is the boundary condition associated with zero gravity surface tension.

In a finite domain a relationship between $\kappa$ and $\gamma$ is imposed by the geometry. Integrating (4.43) over the domain and using the divergence theorem gives

$$\kappa = \cos(\gamma) \frac{|\partial \Omega|}{|\Omega|} \quad (4.45)$$

This is the same condition as the existence condition for Poisson’s equation (4.18) with $\cos \gamma$ replaced by $c$. For zero gravity surface tension problems this constraint is due to the fixed volume of fluid used.

The CMC equation is examined because of its structural similarity to the Laplace–Young equation. One advantage of the CMC equation over the Laplace–Young equation for boundary tracing purposes is that there is a larger number of known exact solutions, see Subsection 4.3.2. In particular it is known that spheres and cylinders are solutions to the CMC problem.

Further details of the behaviour of CMC surfaces can be found in Finn’s book on surface tension [8].

**Geometrical Interpretation** The mean curvature, $H$, of a surface $S$ in $\mathbb{R}^3$ is a function $H : S \rightarrow \mathbb{R}$. The value of $H$ at some point on $S$ is the mean of the principle curvatures $k_1$ and $k_2$ at that point.

The principle curvatures of a surface at a point $p$ are the maximum/minimum curvatures at $p$, of the curves through $p$ given by the intersection of $S$ with planes containing the normal to $S$ at $p$. 
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This definition is not restricted to surfaces which project simply onto the $x$-$y$ plane. Also this curvature property is invariant under translations and rotations in three dimensional space.

For projectable surfaces we can express the mean curvature as

$$\nabla \cdot \frac{\nabla \eta}{\sqrt{1 + \nabla \eta^2}} = 2H$$

(4.46)

see Finn [8]

4.3.2 Known Solutions There are a very large number of known results for CMC surfaces. The Delauney surfaces [6] provide all rotationally symmetric solutions and are described in Eells’ article [7]. Wente [32] developed a technique for generating compact CMC surfaces using properties of their Gauss maps. A variety of these CMC surfaces can be seen in Figure 4.36.

Figure 4.36: A variety of CMC surfaces generated by Nicholas Schmitt using his CMCLab program [30].

Infinite families of minimal surfaces can be constructed using the Weierstaß-Enneper immersion formulae, described by Oprea in [26]. These surfaces include the helicoids and catenoids as well as an infinite variety of other surfaces.

As can be seen from Figure 4.36 many of these CMC/minimal surfaces do not project simply onto the $x$-$y$ plane; however this is required for boundary tracing. Projectable solutions can be obtained by restricting ourselves to pieces of these solutions (such as the lower half of a cylinder aligned with the $x$ axis).

Whilst the invariance under three dimensional rotation increases the family of potential solutions dramatically and any projectable section of a CMC surface could theoretically be used for boundary tracing, most are too complicated to be attempted here. We will restrict ourselves to the simplest cases: the cylinder and sphere solutions.
4.3.3 Channel Solution An infinite cylinder of radius $R$, with its axis along the $x$-axis solves the CMC equation (4.43) with $\kappa = 1/R$. The solution is given by

$$\eta(x, y) = H - \sqrt{R^2 - y^2}$$

(4.47)

The constant contact angle boundary conditions (4.44) are satisfied on the lines $y = \pm R \cos \gamma$. Thus the solution within a channel has been constructed.

Boundary tracing provides alternate curves along which the boundary conditions hold.

*Boundary Curves* Assuming that the boundary has the form $y = f(x)$ then the normal to the boundary is given by

$$\hat{n} = \frac{\pm 1}{\sqrt{1 + f'(x)^2}} \begin{bmatrix} f'(x) \\ -1 \end{bmatrix}$$

and the boundary condition becomes

$$\cos \gamma = \frac{\nabla \eta \cdot \hat{n}}{\sqrt{1 + |\nabla \eta|^2}} = \frac{\pm 1}{\sqrt{1 + f'^2}} \begin{bmatrix} 0 \\ f/R \end{bmatrix} \cdot \begin{bmatrix} -f' \\ 1 \end{bmatrix} = \frac{\pm f}{R\sqrt{1 + f'^2}}$$

This can be rearranged to give

$$f'(x)^2 = \frac{f^2}{R^2 \cos^2 \gamma} - 1$$

(4.48)

which can be integrated to give

$$y = \pm R \cos \gamma \cosh \left( \frac{\pm (x - x_0)}{R \cos \gamma} \right)$$

(4.49)

where $x_0$ is an arbitrary constant.

Note that these solutions, shown in Figure 4.37, match smoothly onto the $y = \pm R \cos \gamma$ solutions at $x = x_0$.

*Corner Behaviour* We can construct a domain with a sharp corner by piecing together two of the traced solutions and the straight line solution, as seen in Figure 4.38. The boundaries of this region will still satisfy the desired boundary conditions.

The physical interpretation is that the shape of the meniscus of a fluid in a channel container in low gravity is unchanged by “denting” the side of the container.
Figure 4.37: Two possible boundaries from boundary tracing the channel solution to the constant curvature problem when $R = c = 1$ and $\gamma = \pi/4$. The lines at $y = \pm 1/\sqrt{2} \approx \pm 0.71$ are terminal curves. The lines at $y = \pm 1$ are the maximum extent of the solution $\eta$.

Conventional wisdom may suggest that interesting behaviour may occur near a corner. This case shows the exact opposite; there is no change in behaviour due to the corner.

We can now examine properties of the solution near these corners. Recall that $\nabla \eta \cdot \hat{n} = ||\nabla \eta|| \sin \alpha$, where $\alpha$ is the half opening angle of the corner. Thus the constant contact angle boundary condition implies

$$\frac{y \sin \alpha}{R} = \cos \gamma$$  \hspace{1cm} (4.50)

Rearranging this for $y$ and substituting into the expression for surface height we obtain

$$\eta = H - \frac{1}{\kappa} \sqrt{1 - \frac{\cos^2 \gamma}{\sin^2 \alpha}}$$  \hspace{1cm} (4.51)

at the corner. Similarly we can obtain the slope at the corner giving

$$||\nabla \eta|| = \frac{2 \cos \gamma}{\sqrt{\sin^2 \alpha - \cos^2 \gamma}}$$  \hspace{1cm} (4.52)

Both of these equations are only defined for $|\sin \alpha| \geq |\cos \gamma|$, that is for $\alpha + \gamma \geq \pi/2$. As $\alpha + \gamma \to \pi/2$ the corner approaches the edge of the cylinder. This requirement on $\alpha + \gamma$ may seem restrictive, but it has been shown by Concus and Finn [5] that for corners with $\alpha + \gamma < \pi/2$ no CMC solution can exist.
4.3.4 Sphere Solution The lower half of a sphere of radius $R$ is a solution to the constant curvature problem when $\kappa = 2/R$.

**Traced Boundary Curves** In this case the terminal curve is given by $r = R \cos \gamma$, and $\eta$ is only defined for $r \leq R$. Thus the viable domain is $R \cos \gamma \leq r \leq R$.

Since the sphere solution $\eta = H_0 - \sqrt{R^2 - r^2}$ is radially symmetric we can use the results of Subsection 3.5.4, that is the boundary curves are given by

$$\theta = \theta_0 \pm \int \frac{G \, dr}{r \sqrt{\eta_r^2 - G^2}}$$

where $G = \nabla \eta \cdot \hat{n} = \cos \gamma \sqrt{1 + \eta_r^2}$.

Using $\eta = H_0 - \sqrt{R^2 - r^2}$ and $\eta_r = r / \sqrt{R^2 - r^2}$ in (4.53) and noting that $R \cos \gamma \leq r \leq R$ we obtain

$$\theta = \theta_0 \pm \int \frac{R \cos \gamma}{r \sqrt{r^2 - R^2 \cos^2 \gamma}}$$

$$= \theta_0 + \arcsin(R \cos \gamma / r)$$

This can be inverted to give

$$r \cos(\theta - \theta_0) = R \cos \gamma$$

These are straight lines tangential to the circle $r = R \cos \gamma$. Thus the terminal curve satisfies the boundary conditions and certain polygonal domains can be constructed, similar to those in Subsection 4.2.5.

**Corner Behaviour** Consider a domain constructed from pieces of traced boundary derived from the sphere solution. We can examine the solution behaviour near
a corner of this domain. From the boundary condition we obtain

\[ \sin \alpha = G / \|
abla \eta \| = \frac{R \cos \gamma}{r} \]

This shows that since \( R \cos \gamma \leq r \leq R \) only angles \( \alpha \) between \( \pi/2 \) and \( \pi/2 - \gamma \) can be constructed. It turns out that this is not correct as convex angles can also be constructed. This gives the entire range of angles, \( \pi/2 - \gamma < \alpha < \pi/2 + \gamma \), for which solutions can exist.

Since the height is given by

\[ \eta = H_0 - \sqrt{R^2 - r^2} \]

\[ = H_0 - R \sqrt{1 - \frac{\cos^2 \gamma}{\sin^2 \alpha}} \]

we see that the height in the corner depends not only on the boundary condition but also the PDE parameters (through \( R \)) and an arbitrary parameter \( H_0 \).

Conversely the slope in the corner is

\[ \eta_r = \frac{r}{\sqrt{R^2 - r^2}} \]

\[ = \frac{\cos \gamma}{\sqrt{\sin^2 \alpha - \cos^2 \gamma}} \]

which depends only on the corner geometry.

It is interesting that the parameter \( \cos \gamma / \sin \alpha \) occurs in both expressions and we will see this occurring again with the Laplace–Young equation in Chapter 6.

**Polygonal Domains** It can be seen that a polygon admits a spherical cap solution with radius \( R \) if all sides (or their extensions) are tangential to an inner circle of radius \( r \) centered on some point \( p \). The minimum radius for the spherical cap is then the maximum distance between \( p \) and the vertices.³

This can be interpreted as follows. Given a polygonal container with all sides tangential to an inner circle of radius \( r \) and all vertices falling inside an outer circle of radius \( R \) both with the same center, then the fluid will form a spherical cap. The contact angle, \( \gamma \), on the container edges is given by \( \cos \gamma = r / R \).

**Example 15.** Equilateral triangles, with side length \( L \), will admit spherical cap solutions when \( \gamma < \pi/3 \). The spherical cap has radius \( R = \frac{\sqrt{3}L}{2 \cos \gamma} \).

Examples of when a solution does and does not exist can be seen in Figure 4.39.

³This condition is essentially that the polygon must also fit entirely inside the sphere.
4.4 Conclusion

The initial examples in this chapter demonstrated the great variety of domains obtainable through boundary tracing. The techniques developed in Chapter 3 were easy to apply and produced sensible results.

The applications to Poisson's equation and the CMC equation showed that the technique can produce interesting and potentially useful information in both linear and nonlinear PDE contexts. In particular it was seen that using boundary tracing on solutions in simple domains (circles or channels) can result in new interesting domains such as polygonal domains or domains with corners.

Figure 4.39: Equilateral triangles, with different boundary conditions, derived from a spherical cap (dashed) by boundary tracing. Left: The triangle fits inside the sphere, thus the sphere is a solution of the CMC problem. Right: The triangle extends beyond the sphere and thus admits no solution.
Helmholtz's Equation

Helmholtz's equation,
\[ \nabla^2 \eta = K \eta, \] (5.1)
is a commonly occurring equation in mathematical physics, often associated with wave propagation problems (with \( K < 0 \)), where it describes the spatial distribution of the propagating field.

In the context of the present work, Helmholtz's equation occurs as a small amplitude approximation of the Laplace-Young equation (with \( K > 0 \)), useful for determining the height rise of liquids for contact angles close to \( \pi/2 \). This approximation has been considered by Fowkes and Hood [11]. In this case the appropriate boundary condition is the linearisation of the constant contact angle boundary condition used for the Laplace-Young equation.

\[ \nabla \eta \cdot \hat{n} = c, \] (5.2)

with \( c = \cos \gamma \).

Since the primary use of Helmholtz's equation in this thesis is for comparison with the Laplace-Young equation, this chapter will assume \( K = \kappa^2 > 0 \). The results obtained in this chapter are similar to those obtained for the Laplace-Young equation in Chapter 6, with any notable differences emphasised in that chapter.

One of the advantages of Helmholtz's equation is the availability of a large variety of exact results which can be used for boundary tracing. We will use boundary tracing on various symmetric cases and will use other exact solutions for comparison purposes.

The divergence theorem allows us to derive properties of "well-behaved" solutions over bounded smooth domains, as it did for Poisson's equation in Section 4.2.1. In this case the mean solution height in the domain satisfies
\[ \bar{\eta} = \frac{c |\partial \Omega|}{K |\Omega|}. \] (5.3)

This does not restrict the choices of \( \Omega, c \) and \( \kappa \) as it did for Poisson's equation and the constant mean curvature equations in Chapter 4, instead providing useful information about the solution.

5.1 Important Known Results

The equations (5.1) and (5.2) have known exact solutions in a variety of domains. These include elementary solutions in the half-plane and channel, and Bessel func-
tion solutions interior and exterior to a cylinder. The solution in a wedge can be expressed in terms of elementary functions for some angles.

Solutions with translational or radial symmetry are introduced as they are used for boundary tracing in Sections 5.2, 5.3 and 5.4. Solutions in wedge shaped domains are compared with solutions in new domains with corners obtained by boundary tracing. In Chapter 7 boundary tracing is used on solutions in wedge shaped domains leading to results concerning rounded corners.

5.1.1 Symmetric Solutions

Half-plane and Channel Solutions Assuming that the solution to (5.1) and (5.2) is independent of $x$ we obtain

$$\eta = Ae^{\kappa y} + Be^{-\kappa y} \quad (5.4)$$

The solution in the half plane $y > 0$ with boundary conditions $\nabla \eta \cdot \hat{n} = c$ on $y = 0$ and $\eta$ bounded as $y \to \infty$ is

$$\eta = \frac{c}{\kappa} e^{-\kappa y} \quad (5.5)$$

Similarly the solution with boundary condition (5.2) on $y = 0$ and $y = y_0$ is given by:

$$\eta = \frac{c \cosh(\kappa(y - y_0/2))}{\kappa \sinh(\kappa y_0/2)} \quad (5.6)$$

Radial Solutions The radially symmetric solutions to (5.1) is

$$\eta = AK_0(\kappa r) + BI_0(\kappa r). \quad (5.7)$$

Here $I_0(r)$ and $K_0(r)$ are the modified Bessel functions of first and second kinds of order 0 respectively. $I_0(r) \to 0$ as $r \to \infty$ and $K_0(r) \to \infty$ as $r \to 0$.

Using this we can obtain the solution inside a cylinder of radius $R$ with bounded behaviour at the origin. This solution is

$$\eta = \frac{cI_0(\kappa R)}{\kappa I_1(\kappa R)} \quad (5.8)$$

An example solution can be seen in Figure 5.1.

Similarly a solution on the exterior of a cylinder with bounded behaviour as $r \to \infty$ is

$$\eta = \frac{cK_0(\kappa R)}{\kappa K_1(\kappa R)} \quad (5.9)$$

The solution in an annular region, between $R_1$ and $R_2$ can be shown to be

$$\eta = \frac{c}{\kappa} \left( \frac{I_1(\kappa R_1) + I_1(\kappa R_2)K_0(\kappa r) + (K_1(\kappa R_1) + K_1(\kappa R_2))I_0(\kappa r)}{K_1(\kappa R_1)I_1(\kappa R_2) - K_1(\kappa R_2)I_1(\kappa R_1)} \right) \quad (5.10)$$
5.1. Important Known Results

5.1.2 Wedge Solutions In Sections 5.2 and 5.3 boundary tracing is used on the the half-plane and channel solutions respectively, to obtain height and slope values at a sharp corner. The analytic results in a wedge provide a useful comparison.

In Chapter 7, boundary tracing is used to examine the effect of corner rounding on height rise using these wedge solutions.

Fowkes and Hood [11] have shown that the solution to (5.1) and (5.2) inside a wedge with half angle $\alpha$ can be expressed in integral form

$$v(r, \theta) = -\frac{2c}{\kappa \pi} \int_{0}^{\infty} \frac{\sinh(\pi \lambda/2)}{\sinh(\alpha \lambda)} K_{\lambda}(\kappa r) \cosh(\lambda \theta) \, d\lambda$$

This solution is derived by separation of variables in radial coordinates and the Kantorovich-Lebedev transformation.

The height, $h$, and slope, $\eta_\varphi$, in the corner are given by

$$h = \frac{c \pi}{2 \kappa \alpha}$$

$$\eta_\varphi = -\frac{c}{\sin \alpha}$$

For certain angles, $\alpha = \frac{\pi}{2n}$, the solution in a wedge can be obtained by the method of images. In these cases (5.11) reduces to a finite sum of exponentials [11]. These solutions are

$$\eta(r, \theta) = \frac{c}{\kappa} \left( e^{-\kappa r \sin(\alpha-\theta)} + e^{-\kappa r \sin(\alpha+\theta)} + e^{-\kappa r \sin(3\alpha-\theta)} + e^{-\kappa r \sin(3\alpha+\theta)} + \ldots + e^{-\kappa r \sin(\pi/2-\theta)} \right)$$
One of the simplest cases is the solution in a right angled wedge. In this case the solution can be written \( \eta = \frac{\varepsilon}{k} (e^{-kx} + e^{-ky}) \) after a simple change of coordinates. This solution can be seen in Figure 5.2.

![Three dimensional plot of solution height in a right angled corner for Helmholtz’s equation](image)

**Figure 5.2:** Three dimensional plot of solution height in a right angled corner for Helmholtz’s equation

Using the symmetry of the wedge solutions and superposition, in a manner similar to the method of images, we can construct the solution inside a “small” wedge by adding together two wedges of double the angle. The two wedges are rotated so that their lines of symmetry fall on the edges of the “small” wedge. This can be seen in Figure 5.3. More concisely denoting the solution inside a wedge of angle \( \alpha \) by \( \eta^\alpha(r, \theta) \) then for \( \alpha < \pi/2 \)

\[
\eta^\alpha(r, \theta) = \eta^{2\alpha}(r, \alpha + \theta) + \eta^{2\alpha}(r, \alpha - \theta)
\]

(5.14)

This satisfies Helmholtz’s equation due to linearity and it is evident that the boundary conditions hold.

### 5.1.3 Wedges with Discontinuous Boundary Conditions

Geometry with different limiting boundary conditions approaching a corner for the Laplace–Young equation has been examined in some detail by several authors [5, 9, 15]. The application of boundary tracing to this situation for the Laplace–Young equation will be considered in Subsection 6.2.7. The solution for differing boundary conditions on the edges of a wedge are obtained for Helmholtz’s equation. These solutions are
5.1. Important Known Results

Figure 5.3: Superposition of two solutions in wedges of angle $2\alpha$, $A$ and $B$ can be used to construct the solution in a wedge of angle $\alpha$, $C$.

compared with the results obtained by boundary tracing one dimensional solutions in Subsection 5.2.6.

Using techniques similar to those used to derive (5.14), it is possible to derive solutions in wedges with opening angle $\alpha < \pi/2$, with different values of the flux boundary condition on either side of the wedge. If the flux along $\theta = \alpha$ is $A$ and that along $\theta = -\alpha$ is $B$, then the solution is

$$\eta = A\eta^{2\alpha}(r, \theta + \alpha) + B\eta^{2\alpha}(r, \theta - \alpha)$$  \hspace{1cm} (5.15)

where $\eta^{2\alpha}$ is the solution inside a wedge with $\nabla \eta \cdot \hat{n} = 1$ on $\theta = \pm 1$, for the same value of $\kappa$.

The height at the corner of such a wedge is given by

$$h = (A + B)\pi/(4\kappa\alpha)$$ \hspace{1cm} (5.16)

and the slope, $||\nabla \eta||$, in the corner is given by

$$||\nabla \eta|| = \frac{1}{\sin 2\alpha}\sqrt{A^2 + B^2 + 2AB \cos 2\alpha}$$ \hspace{1cm} (5.17)

Clearly (5.15) and (5.17) reduce to the appropriate values (equations (5.12) and (5.13) respectively) when $A = B$.

5.1.4 Further Corner Results For Helmholtz's equation, with the constant flux boundary conditions the slope at a corner is entirely determined by the constant
c and the opening angle\(^1\). This is in contrast to the height in the corner, which is not entirely determined by the local conditions. The following example demonstrates this.

**Example 16.** The solution to Helmholtz’s equation with the boundary condition \(\nabla \eta \cdot \hat{n} = c\) inside a square with side length \(2L\) is

\[
\eta = \frac{c(\cosh(\kappa x) + \cosh(\kappa y))}{\kappa \sinh(\kappa L)}
\]

This is in contrast to the height in the corner, which is not entirely determined by the local conditions. The following example demonstrates this.

Thus the height at the corner is given by

\[
h = \frac{2c}{\kappa} \text{coth}(\kappa L)
\]

which is dependent upon the size of the square. However, the magnitude of the gradient at the corner is given by

\[
g = c\sqrt{2};
\]

which is independent of \(L\).

These results can be interpreted as follows: an accurate approximation to the geometry locally, but not globally, only preserves certain properties. Thus the corner of a domain constructed using boundary tracing has the same slope as the corner of a domain which it approximates locally, whilst the heights in these corners need not match. In practice the solution in the traced domain does, in fact, provide a reasonable estimate of corner behaviour for many cases.

### 5.2 One Dimensional Wall Solution

Using the half plane solution,

\[
\eta = \frac{c}{\kappa} e^{-\kappa y}
\]

new domains with corners can be generated.

#### 5.2.1 Boundary Curves

Since \(\eta\) is a function of \(y\) alone we can use the results of Subsection 3.5.1 to obtain the traced boundaries. The boundary condition \(\nabla \eta \cdot \hat{n} = c\) leads to

\[
x + C = c \int \frac{dy}{\sqrt{c^2 e^{-2\kappa y} - c^2}}
\]

\[
= \int \frac{dy}{\sqrt{e^{-2\kappa y} - 1}}
\]

\(^1\)In fact, in this particular case, the slope is determined by the boundary conditions and the geometry, the PDE plays no role.
This integral can be evaluated to give

\[ y(x) = \frac{1}{\kappa} \ln |\cos(C \pm \kappa x)| \]  

(5.24)

\[ y(x) = \begin{cases} 
0 & \text{for } x < -W \\
\ln \cos(W + x) & \text{for } -W \leq x < 0 \\
\ln \cos(W - x) & \text{for } 0 \leq x < W \\
0 & \text{for } W < x
\end{cases} \]  

(5.25)

for some \( 0 < W < \pi/2 \). This boundary is continuous, with piecewise continuous derivatives and has \( \nabla \eta \cdot \hat{n} = c \) for \( \eta = \frac{\xi}{\kappa} e^{-\kappa y} \). As can be seen in Figure 5.5, the domain has a sharp corner at \((0, \ln \cos W)\).

Note that by adjusting the choice of \( W \), different angles can be obtained at the corner. The behaviour at this corner will be compared with the behaviour near the corner of a complete wedge, with corresponding angle.

5.2.3 Comparison with the Wedge Solution We now have two domains having corners with relatively simple solutions, the wedge solution (5.11) and the solution in the traced domain (5.25). Although the local geometry is similar the
global geometry differs strongly. An indication of the relative effect of global geometry versus local geometry can be obtained by examining how the solution inside the constructed domain differs from the solution inside the wedge. It will be shown that the two are closer than might be expected given the comments in Subsection 5.1.4.

Recall that the height in the corner of the wedge is given by \( H = \frac{c\pi}{2\kappa\alpha} \), and the slope is given by \( c/\sin\alpha \).

Using (3.61) from Section 3.4.3 \( \sin\alpha = e^{\kappa y} \), where \( \alpha \) is the half angle at the corner, or equivalently the angle between the tangent to the traced boundary and the lines of constant \( x \). Thus the height at the corner when the opening angle is \( \alpha \) is given by

\[
\begin{align*}
\text{height} & = \frac{c}{\kappa} e^{-\kappa y} = \frac{c}{\kappa \sin\alpha}. \\
\end{align*}
\]

A comparison of the height with the height in a wedge can be seen in Figure 5.6.

Notice that both cases have height \( c \) when \( \alpha = \pi/2 \) and both have a \( 1/\alpha \) type singularity as \( \alpha \to 0 \). It is easy to see that \( \alpha \approx 0, H/h \approx \frac{\pi}{\kappa} \).

The magnitude of the gradient of the traced solution in the corner is

\[
||\nabla \eta|| = \frac{1}{\sin\alpha}
\]

which is the same value that occurs for the wedge case.

Although the behaviour near the corner is similar for the wedge domain and the traced domain, the solution in the traced domain, \( \eta = \frac{c}{\kappa} e^{-\kappa y} \), is much simpler than the solution in the wedge, (5.11).
5.2. One Dimensional Wall Solution

A comparison of the heights in the corner of a wedge (upper) and the sharp corner generated by boundary tracing (lower) the one dimensional wall solution for Helmholtz’s equation with $c = 1$, $\kappa = 1$

A three dimensional plot of the solution in one of these domains can be seen in Figure 5.7 (See Figure C.6 for colour version). From this we can see important features such as the rise into the corners.

5.2.4 Re-entrant Corners We have constructed domains with convex corners using two pieces of the traced boundary curves. Using four pieces it is possible to construct domains with re-entrant corners. An example of such a domain can be seen in Figure 5.8.

It can be shown in the same manner as before that

$$h = \frac{c}{\kappa \sin \alpha} \tag{5.28}$$

A comparison of this with the height in a re-entrant wedge can be seen in Figure 5.9. Thus we see that for the re-entrant corner the similarity in solution behaviour is less than in the convex case. In contrast, the slope in the corner matches exactly.

A solution in one of these domains can be seen in Figure 5.10 (See Figure C.7 for colour version). This shows that $\eta$ drops in the $y$ direction, moving from the tip of the wedge into the interior of the domain. Moving along the edge of the domain, away from the tip, $\eta$ increases until a second corner is reached after which $\eta$ drops until it reaches the one dimensional wall height.

5.2.5 Rough Surfaces Through repeated use of the traced curves we can construct a “rough surface” made from teeth like pieces, see Figure 5.11 (See Figure C.8 for colour version). These teeth can be made arbitrarily small. A simple measure of the roughness of this surface can be used to determine an effective boundary
Figure 5.7: Image of the three dimensional solution for Helmholtz's equation in a domain with a sharp corner, constructed by boundary tracing. (See Figure C.6 for colour version)

condition for the rough surface. These issues will be examined in greater detail for the Laplace–Young equation in Section 6.4.

The roughness factor, \( \rho \), of a curve is defined to be the ratio of the “microscopic length” of the curve to its “macroscopic length”.

Consider one of these tooth like curves centered around some value of \( y = \bar{y} \). Equation (5.2) requires that the edges of these teeth make an angle of approximately \( \alpha \) with \( \nabla \eta \) where \( \| \nabla \eta \| \sin \alpha = c \). Thus \( e^{-\pi y} = 1/\sin \alpha \). As the teeth get smaller, their edges becomes straighter and the approximation improves. Assuming each

Figure 5.8: Construction of a re-entrant corner: The dark lines are domain boundary, the grey lines the full traced boundaries.
5.2. One Dimensional Wall Solution

Figure 5.9: Height in the corner of a domain constructed from traced boundaries and in a wedge. Re-entrant corner are $\alpha > \pi/2$.

tooth has width $W$ then the length of the curve making up the edge of the tooth is approximately $W/\sin \alpha$. Over $n$ teeth the “macroscopic” length is $nW$ and the “microscopic” length is $nW/\sin \alpha$. The ratio of these lengths gives $\rho = 1/\sin \alpha = e^{-\kappa\tilde{y}}$.

Next we look at the behaviour of $\eta$ near $\tilde{y}$, using $Y = y - \tilde{y}$. The solution $\eta = \zeta e^{-\nu}$ becomes

$$\eta = \frac{c e^{-\kappa\tilde{y}}}{\kappa} e^{-\kappa Y}$$  \hspace{1cm} (5.29)

Now since $e^{-\kappa\tilde{y}} = \rho$ so

$$\eta = \frac{c\rho}{\kappa} e^{-\kappa Y}$$  \hspace{1cm} (5.30)

which is the solution in the domain $Y > 0$ with the boundary condition $\nabla \eta \cdot \hat{n} = c\rho$ on $Y = 0$.

Thus the macroscopic effect of introducing the microscopic teeth into the boundary is to change the effective boundary condition from $\nabla \eta \cdot \hat{n} = c$ to $\nabla \eta \cdot \hat{n} = c\rho$, where $\rho$ is the roughness of the new boundary.

Note that a similar procedure can be used on other geometry. Roughening the boundary of some domain by a factor of $\rho$ changes the boundary condition from $\nabla \eta \cdot \hat{n} = c$ to $\nabla \eta \cdot \hat{n} = \rho c$, which changed the solution height in the domain from $\eta$ to $\rho \eta$.

While the curves used for roughening the boundary are special curves produced from boundary tracing the results show that if a relationship between the roughness
factor, $\rho$, and the effective boundary condition exists, then it must be the one derived here.

5.2.6 Differing Boundary Constants Using the solution $\eta = \kappa^{-1}e^{-\kappa y}$ we can trace boundaries for different choices of $c$ in the boundary condition $\nabla \eta \cdot \hat{n} = c$. Pieces of these traced boundaries can be joined together to obtain a corner with different boundary conditions on either side of the vertex. An example of this can be seen in Figure 5.12 (See Figure C.9 for colour version)

With the solution $\eta = \kappa^{-1}e^{-\kappa y}$, there are boundaries with boundary condition $\nabla \eta \cdot \hat{n} = c_1$. In particular these boundaries are

1. The straight line $y = -\kappa^{-1}\ln c_1$
2. The curved boundary $y = \kappa^{-1}(\ln |\cos(C \pm \kappa x)| - 1/\ln c_1)$

Consider following one of these traced boundaries and examining the angle, $\theta$, between the tangent and $\nabla \eta$. The boundary condition requires $\|\nabla \eta\| \cdot \|\hat{n}\| \sin \theta = c_1$. 
5.2. One Dimensional Wall Solution

Figure 5.11: Image showing a “rough” surface and solution produced by boundary tracing. Grey lines in the left figure are full traced boundary curves. (See Figure C.8 for colour version)

Thus

\[ \sin \theta = \frac{c_1}{\| \nabla \eta \|} \]

\[ = c_1 e^{k \eta} \]

\[ = \frac{c_1}{\kappa} \eta^{-1} \]

Two traced boundaries with different boundary conditions can intersect. Then there will be two different angles, \( \alpha_1 \) and \( \alpha_2 \), formed between their tangents and \( \nabla \eta \) at their point of intersection. These intersections can occur in four different ways, see Figure 5.13.

Only the first case in Figure 5.13 will be examined as the other cases are similar. Here the opening angle of the corner is given by \( \alpha = \frac{\alpha_1 + \alpha_2}{2} \). We want to obtain the height in the corner, \( h \), as a function of \( \alpha \) and the two boundary conditions. Using
Figure 5.13: The four ways that two traced boundaries with different boundary conditions can cross. The ellipses surround the vertices of interest.

\[
\sin(\alpha_1) = \frac{c_1}{(\kappa h)} \quad \text{and} \quad \sin(\alpha_2) = \frac{c_2}{(\kappa h)}
\]
we obtain

\[
\cos(2\alpha) = \cos \alpha_1 \cos \alpha_2 - \sin \alpha_1 \sin \alpha_2
\]

\[
\kappa^2 \cos(2\alpha) h^2 = \sqrt{\kappa^2 h^2 - c_1^2 \kappa^2 h^2 - c_2^2 - c_1 c_2}
\]

Solving this for \( h \) gives

\[
h = \frac{1}{\kappa \sin 2\alpha} \sqrt{c_2^2 + c_1^2 + 2c_1 c_2 \cos 2\alpha}
\]

which for small \( \alpha \) gives

\[
h \approx \frac{c_1 + c_2}{2\kappa \alpha}
\]

In Subsection 5.1.3 it was shown that the height in a wedge with differing boundary conditions was \( H = (c_1 + c_2) \pi/(4\kappa \alpha) \). Thus \( H/h \approx \pi/2 \) for small \( \alpha \). This is the same ratio that occurred in Subsection 5.2.3.

Since \( \eta = \kappa^{-1} e^{-\kappa y} \), at any point the slope is given by

\[
\|\nabla \eta\| = e^{-\kappa y} = \kappa \eta
\]

Thus for traced boundaries the slope in the corner is

\[
\|\nabla \eta\| = \frac{1}{\sin 2\alpha} \sqrt{c_2^2 + c_1^2 + 2c_1 c_2 \cos 2\alpha}
\]

which is the same as that derived in Subsection 5.1.3.
5.2.7 Numerical Validation

Some doubts have been raised about the stability of the solutions in these special traced domains to small changes in boundary geometry. Also the question of whether they denote physical solutions have been raised. These doubts can be eased by simple numerical validation.

Helmholtz's equation was solved numerically, using finite elements, in the domain

\[
\begin{cases}
0 & \text{for } x < -\pi/4 \\
\ln \cos(x + \pi/4) & \text{for } -\pi/4 < x < 0 \\
\ln \cos(x - \pi/4) & \text{for } 0 < x < \pi/4 \\
0 & \text{for } \pi/4 < x
\end{cases}
\]

The exact solution, obtained by boundary tracing, in the domain is \( e^{-y} \). The maximum error between the calculated solution and the exact solution was found to be less than 0.01. The solution and the error can be seen in Figure 5.14 (See Figure C.10 for colour version).

This demonstrates that the solutions produced by boundary tracing are physical solutions. Also since the solution was obtained on a relatively coarse grid using linear triangular elements, the solutions in traced domains are not unusually sensitive to perturbations of the boundary.
5.3 Channel 1-D Solution

Here boundary tracing is used on the channel solution of Subsection 5.1.1. This solution is

$$\eta = \frac{c \cosh \kappa y}{k \sinh \kappa L}$$  \hspace{1cm} (5.35)

with the boundary condition $\nabla \eta \cdot \hat{n} = 1$ on $y = \pm L$. Note that

$$\eta_y = \frac{c \sinh \kappa y}{\sinh \kappa L}$$  \hspace{1cm} (5.36)

so

$$\kappa^2 \eta - \eta_y^2 = \frac{c^2}{\sinh^2 \kappa L}$$  \hspace{1cm} (5.37)

which can be solved for $\eta_y(\eta)$ giving

$$\eta_y^2 = \kappa^2 \eta - \frac{c^2}{\sinh^2 \kappa L}$$  \hspace{1cm} (5.38)

Since $\eta_y$ is given as a function of $\eta$ the results of Subsection 3.5.3 can be used. This gives

$$y(\eta) = \int \frac{1}{\eta_y} \, d\eta$$

$$= \int \frac{d\eta}{\sqrt{\kappa^2 \eta^2 - c^2 / \sinh^2 (\kappa L)}}$$

$$= \kappa^{-1} \log(\eta + \sqrt{\eta^2 - c^2 / \sinh^2 (\kappa L)}) + C$$

$$x(\eta) = \int \frac{d\eta}{\eta_y \sqrt{\eta_y^2 - c^2}}$$

$$= \int \frac{d\eta}{\sqrt{\kappa^2 \eta^2 - c^2 / \sinh^2 (\kappa L)} \sqrt{\kappa^2 \eta^2 - c^2 / \sinh^2 (\kappa L)} - c^2}$$

$$= \int \frac{d\eta}{\sqrt{\kappa^2 \eta^2 - c^2 / \sinh^2 (\kappa L)} \sqrt{\kappa^2 \eta^2 - c^2 \cosh^2 (\kappa L)} / \sinh^2 (\kappa L)}$$

$$= \frac{-\sinh (\kappa L)}{c \kappa} \mathcal{F} \left( \text{arcsin} \left( \frac{c}{\eta \kappa \sinh (\kappa L)} \right) \mid \cosh^2 (\kappa L) \right)$$

Both $x$ and $y$ are obtained as parametric functions of $\eta$. Earlier $\eta$ was given as a function of $y$, so we can obtain $x$ as a function of $y$. This gives

$$x = \frac{-\sinh (\kappa L)}{c \kappa} \mathcal{F} \left( \text{arcsin sech}(\kappa y) \mid \cosh^2 (\kappa L) \right) + C$$  \hspace{1cm} (5.39)
5.3. Channel 1-D Solution

We can invert this using the Jacobi Amplitude function to obtain $y$ as a function of $x$

$$y = \pm \kappa^{-1} \arccosh \text{ns} \left( \frac{ck}{\sinh(\kappa L)} (x - C) \big| \cosh^2(\kappa L) \right)$$  \hspace{1cm} (5.40)

where $\text{ns}(a \mid b)$ is a Jacobi elliptic function, see Appendix B. Boundaries for $c = 1$, $\kappa = 1$, $C = -\pi/2$ and $L = 5$ can be seen in Figure 5.15. The $y(x)$ curve has singularities at

$$x = C + \frac{\text{ns}^{-1}(1 \mid \cosh^2(\kappa L))}{ck}$$

Figure 5.15: The traced boundary curves using the solution to Helmholtz’s equation in a channel of width 5.

5.3.1 Corner Behaviour Domains with corners can be constructed in a similar manner to Section 5.2. The height in the corner of these new domains can be derived as follows

$$\eta = \frac{c \cosh(\kappa y)}{\kappa \sinh(\kappa L)}$$ \hspace{1cm} (5.41)

$$\|\nabla \eta\| = c \frac{\sinh(\kappa y)}{\sinh(\kappa L)}$$ \hspace{1cm} (5.42)

$$\nabla \eta \cdot \hat{n} = \|\nabla \eta\| \sin \alpha = c$$ \hspace{1cm} (5.43)

Combining (5.42) and (5.43) gives

$$\frac{\sinh(\kappa y)}{\sinh(\kappa L)} = \frac{1}{\sin \alpha}$$ \hspace{1cm} (5.44)

Squaring this and using $\cosh^2(x) - \sinh^2(x) = 1$ we obtain

$$\frac{\cosh^2(\kappa y)}{\sinh^2(\kappa L)} = \frac{1}{\sin^2 \alpha} + \frac{1}{\sinh^2(\kappa L)}$$ \hspace{1cm} (5.45)
Now using (5.41) and simplifying we obtain the height in the corner as a function of $\alpha$:

$$h = \frac{c}{\kappa} \sqrt{\frac{1}{\sinh^2(\kappa L)} + \frac{1}{\sin^2 \alpha}} \quad (5.46)$$

This differs from the height obtained in the traced domains of the half plane solution (5.26) derived in Subsection 5.2.3, by the inclusion of the $1/\sinh^2(\kappa L)$ term. This term is due to the influence of the far boundary. For large $L$ (5.46) becomes

$$h = h_\infty + \frac{ce^{-\kappa L}}{\kappa h_\infty}$$

where $h_\infty = -\frac{c}{\kappa \sin \alpha}$ is the height for the traced half-plane domains with the same wedge angle. Thus the effect of the far boundary is exponentially decreasing with $L$ and $h \to h_\infty$ as $L \to \infty$, as expected.

In a similar manner we can obtain the slope in the corner. In this case the values match those for traced boundaries in the half-plane and the wedge case.

### 5.4 Radial Tracing

In this section traced boundaries for radial solutions to Helmholtz’s equation are found. The integrals which arise cannot be expressed in terms of standard functions, so the boundaries are calculated numerically.

The radial solution for Helmholtz’s equation which is bounded as $r \to \infty$ is

$$\eta = AK_0(\kappa r) \quad (5.47)$$

Then $\eta_r$ is given by

$$\eta_r = -K_1(r) \quad (5.48)$$

Now due to the symmetry we can use the results of Subsection 3.5.4. This gives

$$\theta + \phi = \pm c \int \frac{dr}{r \sqrt{A^2 \kappa^2 K_1(\kappa r)^2 - c^2}} \quad (5.49)$$

A graph of this function can be seen in Figure 5.16.

Helmholtz’s equation admits simple radial solutions in annular domains given by $\eta = AK_0(r) + B I_0(r)$. Boundary tracing with these solutions numerically gives rise to unusually shaped domains. The traced boundaries for $\eta_1 = K_0(r), \eta_2 = I_0(r)$ and $\eta_3 = \frac{3}{2} K_0(r) + I_0(r)$ are shown in Figure 5.17. The inner white circles of the $\eta_1$ and
5.5 Conclusion

In this chapter boundary tracing provided alternate derivation/verification of various results for Helmholtz's equation and developed a variety of new results. These included determining the effect of far field geometry on corner behaviour by boundary tracing the channel solution, construction of domains with "rough" boundaries and determining solution behaviour near corners with differing boundary conditions on either side of the corner.

While these results are of interest on their own, that they were obtained easily demonstrates boundary tracing's utility.

Figure 5.16: The result of boundary tracing on the singular $K_0(r)$ solution to Helmholtz's equation. The inner boundary is the traced boundary.

$\eta_3$ boundaries, are due to truncation of the boundaries and are not terminal curves. This is also the case for the outer circles of the $\eta_2$ and $\eta_3$ cases.

Using these boundaries we can construct a variety of exotic domains with exact solution, such as the "spiky ring" seen in Figure 5.18 (See Figure C.11 for colour version).
Figure 5.17: Traced boundaries for the boundary condition $\nabla \eta \cdot \hat{n} = 1$ with $\eta_1 = K_0(r)$, $\eta_2 = I_0(r)$ and $\eta_3 = \frac{3}{2}K_0(r) + I_0(r)$.

Figure 5.18: Left: An annular solution to Helmholtz's equation, with its traced counterpart. Note the height rise into the corners. Right: The two solutions match together smoothly. (See Figure C.11 for colour version)
The Laplace–Young Equation

The Laplace–Young equation determines the equilibrium height, \( \eta \), of the free surface of a liquid in a container under the influence of gravity and surface tension. Derivations of the equation can be found in Finn’s book [8] and Landau & Lifshitz [16].

In scaled form the Laplace–Young equation is

\[
\nabla \cdot \frac{\nabla \eta}{\sqrt{1 + |\nabla \eta|^2}} = \eta
\]

(6.1)

The physically appropriate boundary conditions are the contact conditions

\[
\frac{\nabla \eta}{\sqrt{1 + |\nabla \eta|^2}} \cdot \hat{n} = \cos \gamma
\]

(6.2)

where \( \gamma \) is the contact angle determined by the properties of the boundary, the lower fluid and the upper fluid (which is typically air), see Figure 6.1.

Figure 6.1: The contact angle \( \gamma \).

The only known exact solutions to the Laplace–Young equation are the two one-dimensional solutions, those in an infinite half plane and in a doubly infinite channel and the zero solution when \( \gamma = 0 \). Asymptotic solutions have been found interior and exterior of a cylinder by Finn [8] and Lo [17] respectively.

In this chapter new domains with exact solution are derived. These are the first known exact domains with sharp corners. They allow the demonstration of a wide variety of known asymptotic results, including slope and height behaviour near a corner.

Finn [8] proved that it is not necessary for an inner domain contained within an outer domain, both with the same boundary condition, to have globally higher solution. Traced boundaries provide a simple example of a stronger result: it is possible for an inner domain to have globally lower solution than an outer domain.

Information concerning the effect of rough boundaries on solutions to the Laplace–Young equation is also obtained. The rough boundaries examined are the limits
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of families of domains with known solutions, each produced by boundary tracing. These domains show that microscale surface roughness causes a simple modification to the boundary condition. This new boundary condition is also supported by energy based arguments independent of boundary tracing.

Non-radially symmetric domains which admit radially symmetric solutions are also generated.

6.1 Known Results

6.1.1 Exact Solutions There are known exact solutions in only three cases:

1. When the contact angle is $\gamma = \frac{\pi}{2}$ the boundary condition becomes $\frac{\nabla \eta \cdot \hat{n}}{\sqrt{1 + \nabla \eta^2}} = 0$, so that $\eta = 0$ is the solution.

2. The solution in the half plane $y > 0$ with the boundary condition (6.2) on $y = 0$ is given by the implicit form

$$y = \cosh^{-1}(2/\eta) - (4 - \eta^2)^{1/2} + C_1$$

for some $C_1$, see Landau and Lifshitz [16].

3. The solution in a channel $-L < y < L$ can be expressed using elliptic functions [16]. See Section 6.3 for further details.

6.1.2 Corner Behaviour The solution behaviour in a corner is known to depend strongly on the half opening angle of the corner, $\alpha$, and the contact angle, $\gamma$. In particular, there is a critical value for $\alpha$, $\alpha_c = \pi/2 - \gamma$, such that for $\alpha < \alpha_c$ the solution in the corner has a singularity, and for $\alpha_c < \alpha < \pi/2$ the solution is locally planar.

The asymptotic behaviour of the solution near a corner is given by:

1. For angles $\alpha < \alpha_c$: The height at the corner is unbounded, having a $1/r$ type singularity. In fact it has been shown that there exists an $A > 0$ such that

$$|\eta - \frac{\cos \theta - (k^2 - \sin^2 \theta)^{1/2}}{kr/l_c^2}| < \frac{A r^2}{l_c^2}$$

where $k = \frac{\sin \alpha}{\cos \gamma}$ and $l_c = \sqrt{\sigma/\rho g}$, for $r < r_0$. See [2, 11, 24, 31].

2. For angles $\alpha_c < \alpha < \pi/2$: In this case the solution is locally planar with

$$\eta = \eta_0 - \frac{x}{\sqrt{k^2 - 1}} + o(r)$$

see Miersemann [23].
3. For re-entrant corners with $\pi/2 < \alpha < \pi - \alpha_c$: King, Ockendon and Ockendon [13] state that the problem can admit locally planar solutions. However Korevaar [14] has constructed examples where the solution does not extend continuously to the vertex.

4. For re-entrant corners with $\pi - \alpha_c < \alpha < \pi$: In this case there are no locally planar solutions to the PDE. King et al. [13] have shown that for symmetric solutions, there are separate regions with different behaviour near the vertex. These regions are based on the straight line characteristics of the steep-slope approximation,

$$\nabla \cdot \frac{\nabla \eta}{||\nabla \eta||} = 0.$$

(6.6)

Korevaar [14] has shown that solutions exist where the solution does not extend continuously to the corner.

5. For the special case $\alpha = \alpha_c$: The behaviour in the case where $\alpha \approx \alpha_c$ has been examined by King et al. [13]. It is shown that as $r \to 0$

$$\eta \to \eta_0 - 2x^{1/2}/\sqrt{\eta_0}$$

(6.7)

for some constant $\eta_0$ which is determined by far field conditions.

6. For the special case $\alpha = \pi/2 + \gamma$: King et al. [13] have shown that for $\alpha = \pi/2 + \gamma$ as $r \to 0$

$$\eta \approx \eta_0 + \frac{x \log |x|}{2\pi \tan \gamma} + O(r)$$

(6.8)

For $\alpha < \alpha_c$ the solution is determined to leading order by (6.4). However for $\alpha_c < \alpha < \pi/2$ the solution is locally planar with only the slope determined locally by (6.5). Thus as $\alpha - \alpha_c$ switches from positive to negative the importance of behaviour determined by the local geometry switch from second order (slope of the locally planar solution) to first order (the nature of singularity of singular solution).

A similar dependence on $\alpha - \alpha_c$ occurred with the CMC solutions in Section 4.3. When $\alpha - \alpha_c$ is positive, solutions can exist, are locally planar with locally determined slope. If $\alpha - \alpha_c$ is negative at any vertex then the solution cannot exist. These are in contrast to Chapter 5 where for Helmholtz's equation the solution existed, was locally planar and had locally determined slope at corners for all values of $\alpha$.

Due to the elliptic nature of the Laplace–Young equation the local behaviour of the solution depends upon the geometry of the entire domain, meaning that local
results generated by boundary tracing may have minimal applicability to general situations. However, guided by the success of the method for Helmholtz's equation in Chapter 5, where the same problems occurred, it is conceivable that boundary tracing will lead to sensible and useful results for the Laplace–Young equation. Also the generation of new domains with known solutions is interesting in its own right.

### 6.2 One Dimensional Wall Solution

The boundary tracing results presented here are derived from the known one-dimensional solutions to the Laplace–Young equation. Details of the derivation of this solution can be found in Landau and Lifshitz [16].

The two known solutions will be called the **wall** solution and the **channel** solution. The wall solution is defined in the region $y > y_0$ for some $y_0$, with the contact condition (6.2) on $y = y_0$. The channel solution is defined in a strip $y_0 < y < y_1$ with the contact conditions on $y = y_0$ and $y = y_1$.

The channel solution will be considered in Section 6.3. For the moment we will restrict our attention to the wall solution.

In one dimension the Laplace–Young equation reduces to the non-linear ODE

$$\frac{d}{dy} \frac{\eta_y}{\sqrt{1 + \eta_y^2}} = \eta$$  \hspace{1cm} (6.9)

Assuming that the height and slope tend toward zero at infinity this can be integrated to give the implicit formula

$$y = \cosh^{-1}(2/\eta) - (4 - \eta^2)^{1/2} + C_1$$ \hspace{1cm} (6.10)

for the surface height, $\eta$, in terms of $y$.

Typically the value of $C_1$ is adjusted so that the desired boundary condition is satisfied on $y = 0$. In this thesis it is convenient to choose $C_1$ such that the singularity in $\eta$ occurs at $y = 0$. This gives $C_1 = \sqrt{2} - \cosh^{-1}(\sqrt{2})$, so that

$$y = \cosh^{-1}(2/\eta) - (4 - \eta^2)^{1/2} - \cosh^{-1}(\sqrt{2}) + \sqrt{2}$$ \hspace{1cm} (6.11)

A parametric plot of this function can be seen in Figure 6.2. It can be seen that the inverse, $\eta(y)$, has two branches. Only the lower branch of the curve, with $\eta < \sqrt{2}$ is used.

Using a Computer Algebra System, such as Mathematica it can easily be shown that for large $y$,

$$\eta(y) \approx K e^{-y}.$$ \hspace{1cm} (6.12)
where $K = \frac{4e^{-2+\sqrt{2}}}{1+\sqrt{2}} \approx 0.922318$. This approximation is a solution to Helmholtz’s equation. Similarly for $0 < y \ll 1$,

$$\eta(y) \approx 2^{1/2} - 2^{1/4}y^{1/2}. \quad (6.13)$$

provides an approximation to the solution. This result will be used later, in Subsection 6.2.5. A comparison of these asymptotic results with the exact result can be seen in Figure 6.3.

For the wall solution the boundary condition (6.2) is satisfied on the line $y = y_0$, 

---

**Figure 6.2:** The solution to the Laplace–Young equation in a half-plane $\eta(y)$.

**Figure 6.3:** A comparison of $\eta(y)$ (solid) with the asymptotic behaviour $Ke^{-y}$ (dotted) and $2^{1/2} - 2^{1/4}y^{1/2}$ (dashed).
where
\[ y_0 = \text{arccosh}\left(\frac{\sqrt{2}}{\sqrt{1 - \sin(\gamma)}}\right) - \text{arccosh}(\sqrt{2}) - \sqrt{2}\left(\sqrt{1 + \sin(\gamma)} - 1\right) \] (6.14)

6.2.1 Boundary Curves As \( \eta \) is given implicitly as a function of \( y \) the results of Subsection 3.5.2 can be used. These give the traced boundaries as

\[ x(\eta) = C \pm \int \frac{Gy'}{\sqrt{1 - G^2y'^2}} d\eta \]

where \( G = \cos \gamma \frac{\sqrt{1 + (y')^2}}{|y'|} \) giving

\[ x(\eta) = K \pm \cos \gamma \int \frac{y'\sqrt{1 + y'^2}}{\sqrt{\sin^2 \gamma - \cos^2 \gamma y'^2}} d\eta \]

Now using
\[ y'(\eta) = \frac{-2 + \eta^2}{\eta \sqrt{4 - \eta^2}} \] (6.15)

we obtain
\[ x = \pm 2 \cos \gamma \int \frac{\eta^2 - 2}{\eta \sqrt{\sin^2 \gamma - \cos^2 \gamma}} \frac{d\eta}{\eta \sqrt{4 - \eta^2}} \] (6.16)

This integral can be evaluated using elliptic integrals giving the boundary parametrically as

\[ x(\eta) = C_1 \pm \frac{\sqrt{2} \cos \gamma}{\sqrt{1 - \sin \gamma}} \left[ \text{F}\left(\sin^{-1}\left(\frac{2 + 2 \sin \gamma - \eta^2}{4 \sin \gamma}\right)|\frac{-2 \sin \gamma}{1 - \sin \gamma}\right) - \frac{1}{1 + \sin \gamma} \Pi\left(\frac{2 \sin \gamma}{1 + \sin \gamma}; \sin^{-1}\left(\frac{2 + 2 \sin \gamma - \eta^2}{4 \sin \gamma}\right)|\frac{-2 \sin \gamma}{1 - \sin \gamma}\right)\right] \] (6.17)

\[ y(\eta) = \cosh^{-1}(2/\eta) - (4 - \eta^2)^{1/2} - \cosh^{-1}(\sqrt{2}) + \sqrt{2} \] (6.18)

Examples of these boundaries for \( \gamma = \pi/4 \) can be seen in Figure 6.4.

These results allow the construction of new domains with exact solutions to the Laplace-Young equation.

6.2.2 Traced Boundary Geometry From the boundary equations (6.17) and (6.18) it can be seen that the boundary only exists for \( \sqrt{2} - 2 \sin \gamma \leq \eta \leq \sqrt{2} \). This corresponds to the region \( y_0 \geq y \geq 0 \), a region of finite width depending on \( \gamma \). This means that for a given \( C \), \( x \) will only take values between \( x(\sqrt{2}) \) and \( x(\sqrt{2} - 2 \sin \gamma) \). Let

\[ W(\gamma) = x(\sqrt{2}) - x(\sqrt{2} - 2 \sin \gamma) \] (6.19)
Then \( W(\gamma) \) is half the maximum width for a simple indent\(^1\) into a surface that does not change the solution behaviour, see Figure 6.5. This is graphed, as a function of \( \gamma \) in Figure 6.6. It can be seen that \( W(\gamma) \approx \gamma \). In fact \( |W(\gamma) - \gamma| < 0.1 \) for \( 0 \leq \gamma \leq \pi/2 \). The maximum intrusion depth is \( y_0(\gamma) \), see Figure 6.5, plotted in Figure 6.7.

Note that as \( \gamma \) approaches \( \pi/2 \) the intrusion depth becomes arbitrarily deep, while the intrusion width approaches \( \pi/2 \). Recall that for Helmholtz's equation the maximum intrusion width was \( \pi/2 \), with unlimited depth. Thus the behaviour of the Laplace-Young equation is consistent with Helmholtz's equation as \( \gamma \to \pi/2 \), as expected.

\(^1\)That is an indent where the two edges of the indent are monotonic.
The angle in the corner approaches $\alpha_c$ as the corner approaches the singularity in the $\eta$ solution. Thus the solution provided here gives a domain with a sharp corner over all values of $\alpha$ where locally bounded planar solutions can be found, that is $\alpha_c \leq \alpha < \pi/2$.

A large variety of more complicated boundary geometries can be constructed all having the same solution. Examples can be seen in Figure 6.8. Similar surfaces will be used in the investigation of rough surfaces in Section 6.4.

Note: It is interesting that a large range of boundaries exist, all generating the same solution. These boundaries cannot be distinguished by their solution behaviour, all being equivalent to a flat wall. This observation underlies the work on rough surfaces in Section 6.4.

6.2.3 Behaviour in the Corner The height in the corner of the traced boundary can be expressed as a function of the contact angle $\gamma$ and the half opening angle of the corner.
6.2. One Dimensional Wall Solution

Figure 6.8: A variety of boundaries constructed by boundary tracing, all with the same solution to the Laplace–Young equation as the half-plane (dotted boundary).

\[
\sin \alpha = \cos \gamma \sqrt{\| \nabla \eta \|^{-2} + 1} \quad \text{from (3.4)} \quad (6.20)
\]

\[
k = \frac{\sin \alpha}{\cos \gamma} = \sqrt{\frac{\eta^2(4 - \eta^2)}{(\eta^2 - 2)^2} + 1} \quad \text{using (6.15)} \quad (6.21)
\]

\[
\eta = \sqrt{2} \sqrt{1 - \sqrt{1 - k^{-2}}} \quad \text{using } 0 < \eta < \sqrt{2}. \quad (6.22)
\]

A graph of \( \eta \) as a function of \( k \) can be seen in Figure 6.9. For \( \gamma \approx \pi/2, \ k \gg 1 \) and \( \eta \approx k^{-1} = \frac{\cos \gamma}{\sin \alpha} \). Boundary tracing for Helmholtz’s equation gave \( H = c/\sin \alpha \) (5.26), thus the solutions are again consistent for \( c = \cos \gamma \ll 1 \).

Figure 6.9: Height, \( \eta \), at the corner of a traced wedge as a function of \( k = \sin \alpha / \cos \gamma \).

Although the slope in the corner is the same as that for an infinite wedge\(^2\) we cannot expect the height to match. This was also the case for Helmholtz’s equation, but it was shown that the height was indeed similar (see Subsection 5.2.3).

\(^2\)This will be shown in Subsection 6.2.4.
To determine how similar the traced solution is to the wedge solution the height in a wedge must be calculated numerically. Solutions in wedges were calculated using a pseudo-time-stepping finite-element method. A comparison between the heights for the traced solutions and numerical simulations for a variety of $\gamma$ and $\alpha$ is shown in Figure 6.10. The numerics includes results for $0 < \alpha < \pi$ and $0 < \gamma < \pi/2$, where $k \geq 1$.

![Figure 6.10: A comparison between the height at a corner for the Laplace–Young equation as a function of $k = \sin \alpha/\cos \gamma$, calculated numerically in a wedge for various choices of $\gamma$ and $\alpha$ (dots), and the analytic result using traced boundaries (curve).](image)

Presumably the differences between the exact solution in the traced corners and the numerical solutions in wedges come from two sources. The first and primary problem is that the geometry differs drastically for points far from the vertex\(^3\) and it is known that the solution behaviour is not determined entirely by local geometry. The second and comparatively minor problem is that there are the usual errors in numerical calculations.

The change due to the differing geometry was noted with Helmholtz's equation in Subsection 5.2.3, where the difference was fairly large over certain angles, especially $\alpha > \pi/2$. It is not surprising that there are the same problems here, where it is well known that the height in a corner can depend strongly on far field geometry.

Numerical errors could also have been introduced, as the numerical scheme used an iterative solution method, which could converge on an aphysical local "minima", rather than global "minima", or appear to have converged when it had not. There is also the usual problems with discretisation errors and the need to impose a boundary condition a finite distance from the origin, rather than at infinity. However these numerical errors were typically small compared to the size of the solution.

\(^3\)One domain being a half-plane far from the origin, the other a wedge.
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In light of the first problem it is surprising that the analytic curve approximates the numerical results as well as it does, clearly falling within the numerical ranges.

6.2.4 Slope in the Corner For the cases with \( \alpha_c < \alpha < \pi/2 \) the surface slope in the corner was obtained by Miersemann [23] and is given by \( \frac{1}{\sqrt{k^2 - 1}} \). As expected the solution given by (6.17) and (6.18) also gives the same result.

\[
\| \nabla \eta \| = \frac{1}{\sqrt{k^2 - 1}}
\]  

(6.23)

For Helmholtz’s equation \( \| \nabla \eta \| = c/\sin \alpha \), which is also the result for the Laplace–Young equation for \( c = \cos \gamma \ll 1 \).

6.2.5 Square Root Singularity For \( \alpha = \alpha_c \) King et al. [13] have shown that as \( \alpha \to \alpha_c \), \( \eta \) approaches a square root singularity at the vertex. In particular

\[
\eta \to \eta_0 - 2x^{1/2}/\sqrt{\eta_0}
\]  

(6.24)

An exact analytic solution in a domain with a corner of angle \( \alpha = \alpha_c \) can be created by patching together pieces of traced boundary.

Equation (6.13) shows that the height near the corner is

\[
\eta = 2^{1/2} - 2^{1/4}y^{1/2}
\]  

(6.25)

While this exhibits the expected singular behaviour, the coefficient of \( x^{1/2} \) appears incorrect. This occurs due to the example having non-zero boundary curvature. In particular, it can be shown that including higher order terms for the boundary geometry changes the equations used to derive the second order behaviour of the solution, equations (14) and (15b), in the article by King et al. [13].

6.2.6 A Simple Counterexample Guided by physical intuition one may expect “small” domains to raise fluid higher than “large” domains. In particular if one domain is inside another, we may expect the solution height inside the interior domain to be higher than the solution in the outer domain at every point. Finn [8] has demonstrated that this expectation is incorrect.

Using boundary tracing we can construct two simple domains, one inside the other, both having the same boundary condition, such that the inner domain has solution which is globally lower than the solution in the outer domain. This counterexample is in many ways superior to that of Finn; not only is the solution in the interior domain lower at some points but it is lower everywhere. Also the approach is of a simple constructional nature.
In more concise notation Finn shows through an elaborate construction that: Given $D_i \subset D_o$ and $\eta_i$ being the solution to (6.1) and (6.2) in $D_i$, and $\eta_o$ the solution in $D_o$, it is not necessary that $\eta_i > \eta_o$ at all points in $D_i$.

Here two nested domains, $D_i \subset D_o$ are determined such that $\eta_i < \eta_o$ at all points in $D_i$.

Using the half-plane solution, construct $D_o$ by boundary tracing a zig-zag boundary $z(x)$, alternating between $y_i$ and $y_u$ where $0 < y_i < y_u < y_o$. Then define $D_o = \{(x,y) | y > z(x)\}$. Thus the solution in $D_o$ is $\eta_o = \eta(y)$.

Next consider the half-plane domain $D_i = \{(x,y) | y > y_h = y_o - h\}$. Where $h$ is chosen so that $y_o > y_o - h > y_u$, and thus $D_i$'s boundary does not intersect $D_o$'s boundary and $h > 0$. It is easy to see that the solution in $D_i$ is $\eta_i = \eta(y + h)$.

The two boundaries are shown in Figure 6.11.

Figure 6.11: Construction of domains $D_i$ and $D_o$ with $\eta_0 > \eta_i$.

Since $\eta(y)$ is a monotonically decreasing function of $y$, it is clear that $\eta(y) > \eta(y + h)$ and consequently $\eta_i < \eta_o$.

Although these domains $D_i$ and $D_o$ are both unbounded, it is possible to obtain the same result for bounded domains using radial solutions.

6.2.7 Differing Boundary Conditions Examinations of the behaviour at a corner with differing boundary conditions on either side of the corner have been done by Lancaster and Siegel [15]. This previous work has shown, among other things, that if $\eta$ is bounded in the neighbourhood of a non-convex corner then the radial limits exist. Also under various conditions (similar to the critical angle condition) the radial limits exist for convex corners.

In particular if $|\pi - \gamma_1 - \gamma_2| < 2\alpha$ and $2\alpha + |\gamma_1 + \gamma_2| \leq \pi$ then $\eta$ is continuous up to the vertex.

Using boundary tracing, exact solutions near a sharp corner with different contact angles on either side of the corner can be constructed. Whilst these boundaries are special the results have wider significance.
Consider the situation presented in Figure 6.12 where two traced boundaries with different contact angles, $\gamma_1$ and $\gamma_2$, meet at a corner.

Figure 6.12: Two traced boundaries with differing contact angles meeting at a corner.

Now along the boundaries

\[
\frac{\|\nabla \eta\| \sin \alpha_1}{\sqrt{1 + \nabla \eta^2}} = \cos \gamma_1 \quad \quad \frac{\|\nabla \eta\| \sin \alpha_2}{\sqrt{1 + \nabla \eta^2}} = \cos \gamma_2
\]

Defining $\bar{k}$ such that

\[
\frac{\nabla \eta}{\sqrt{1 + \nabla \eta^2}} = \bar{k}^{-1}
\]

(6.26)

gives $\sin \alpha_1 = \bar{k} \cos \gamma_1$ and $\sin \alpha_2 = \bar{k} \cos \gamma_2$. Using $2\alpha = \alpha_1 + \alpha_2$ gives

\[
\cos 2\alpha = \cos \alpha_1 \cos \alpha_2 - \sin \alpha_1 \sin \alpha_2
\]

\[
= (1 - \bar{k}^2 \cos^2 \gamma_1)^{1/2} (1 - \bar{k}^2 \cos^2 \gamma_2)^{1/2} - \bar{k}^2 \cos \gamma_1 \cos \gamma_2
\]

Rearranging and solving for $\bar{k}$ gives

\[
\bar{k} = \frac{\sin 2\alpha}{\sqrt{\cos^2 \gamma_1 + 2 \cos \gamma_1 \cos \gamma_2 \sin 2\alpha + \cos^2 \gamma_2}}
\]

(6.27)

Now using $\|\nabla \eta\| = \eta_y = \frac{\eta \sqrt{4 - \eta^2}}{\eta^2 - 2}$ in (6.26) we obtain

\[
\bar{k}^{-1} = \frac{\sqrt{\eta^4 + 2}}{\eta \sqrt{4 - \eta^2}}
\]

(6.28)

Solving (6.28) for $\eta$ and noting that $0 < \eta < \sqrt{2}$ gives the height at the corner as

\[
\eta = \sqrt{2} \sqrt{1 - \sqrt{1 - \bar{k}^{-2}}}
\]

(6.29)
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The result (6.29) is the same result obtained in Subsection 6.2.3 with $k$ replaced with $\tilde{k}$. If $\gamma_1 = \gamma_2 = \gamma$ then $\tilde{k} = \sin \alpha / \cos \gamma$ and the equations become the same.

The slope in the corner can be derived using a similar method, giving

$$\eta_\mu = \frac{-1}{k^2 - 1} \quad (6.30)$$

This is again the result from Subsection 6.2.4 for $\gamma_1 = \gamma_2 = \gamma$ with $k$ replaced by $\tilde{k}$.

Not all angles, $\alpha$, can be obtained in the corner using boundary tracing. We will determine over which range of angles our results hold.

Letting $\gamma_1 > \gamma_2$ then $\pi/2 - \gamma_1 < \alpha_1 < \pi/2$, and using

$$\frac{\|\nabla \eta\|}{\sqrt{1 + \nabla \eta^2}} = \frac{\cos \gamma_1}{\sin \alpha_1} = \frac{\cos \gamma_2}{\sin \alpha_2} \quad (6.31)$$

we obtain

$$\alpha_2 = \sin^{-1}\left(\frac{\cos \gamma_2}{\cos \gamma_2}\sin \alpha_2\right) \quad (6.32)$$

Hence $\pi/2 - \gamma_2 < \alpha_2 < \sin^{-1}(\cos \gamma_2 / \cos \gamma_1)$.

There are four geometrically different cases, as in Subsection 5.1.3:

1. $\alpha = \frac{1}{2}(\alpha_1 + \alpha_2)$: It can be seen that this covers the range

$$\frac{\pi}{2} - \frac{\gamma_1 + \gamma_2}{2} \leq \alpha \leq \frac{\pi}{4} + \sin^{-1}\left(\frac{\cos \gamma_2}{\cos \gamma_1}\right) \quad (6.33)$$

2. $\alpha = \frac{1}{2}(\pi - \alpha_1 + \alpha_2)$: This covers the range

$$\frac{\pi}{4} + \sin^{-1}\left(\frac{\cos \gamma_2}{\cos \gamma_1}\right) \leq \alpha \leq \frac{\pi}{2} - \frac{\gamma_1 - \gamma_2}{2} \quad (6.34)$$

3. $\alpha = \frac{1}{2}(\alpha_1 + \pi - \alpha_2)$:

$$\frac{\pi}{2} - \frac{\gamma_1 - \gamma_2}{2} \leq \alpha \leq \frac{3\pi}{4} - \sin^{-1}\left(\frac{\cos \gamma_2}{\cos \gamma_1}\right) \quad (6.35)$$

4. $\alpha = \frac{1}{2}(2\pi - \alpha_1 - \alpha_2)$:

$$\frac{3\pi}{4} - \sin^{-1}\left(\frac{\cos \gamma_2}{\cos \gamma_1}\right) \leq \alpha \leq \frac{\pi}{2} + \frac{\gamma_1 + \gamma_2}{2} \quad (6.36)$$

Thus the range covered by $\alpha$ is

$$\frac{\pi}{2} - \frac{\gamma_1 + \gamma_2}{2} \leq \alpha \leq \frac{\pi}{2} + \frac{\gamma_1 - \gamma_2}{2} \quad (6.37)$$

$$\frac{\pi}{2} - \frac{\gamma_1 - \gamma_2}{2} \leq \alpha \leq \frac{\pi}{2} + \frac{\gamma_1 + \gamma_2}{2} \quad (6.38)$$

$$\frac{\pi}{2} - \frac{\gamma_1 + \gamma_2}{2} \leq \alpha \leq \frac{\pi}{2} + \frac{\gamma_1 - \gamma_2}{2} \quad (6.39)$$
This is the range of $\alpha$ where the solution is known to be continuous up to the vertex. Thus for all cases where we are guaranteed a locally planar solution, a domain with analytic boundary and solution can be constructed having a corner with the required angle. For these solutions the height and slope in the corner can be expressed in terms of the wedge angle and boundary conditions.

### 6.3 1-D Channel Solution

A derivation of the channel solution is available in Landau and Lifshitz [16]. An equivalent derivation is presented here, as intermediate steps will be used for boundary tracing in Subsection 6.3.1.

Assuming a one dimensional solution, $\eta(y)$, of the Laplace–Young equation we obtain the ODE

$$\frac{\eta_{yy}}{(1 + \eta_y^2)^{3/2}} = \eta$$  \hspace{1cm} (6.40)

Multiplying by $\eta_y$ and integrating gives

$$\frac{1}{1 + \eta_y^2} = A - \frac{1}{2}\eta^2$$  \hspace{1cm} (6.41)

The desired channel is symmetric about $y = 0$ requiring $\eta_y(0) = 0$ so

$$\eta(0) = \sqrt{2}\sqrt{A - 1}$$  \hspace{1cm} (6.42)

Assuming that $\eta_y$ has its singularities at $y = \pm W$, then

$$\eta(W) = \sqrt{2}\sqrt{A}$$  \hspace{1cm} (6.43)

Now solving (6.41) for $\eta_y$, we obtain

$$\frac{d\eta}{dy} = \frac{\sqrt{1 - (A - \eta^2/2)^2}}{A - \eta^2/2}$$  \hspace{1cm} (6.44)

Integrating this by interchanging the independent and dependent variables gives

$$y = \int_{\eta_0}^{\eta} \frac{A - \eta^2/2}{\sqrt{1 - (A - \eta^2/2)^2}} \, d\eta$$  \hspace{1cm} (6.45)

The substitution $A - \eta^2/2 = \cos \phi$ leads to

$$y = \frac{1}{\sqrt{2}} \int_0^\phi \frac{\cos \phi}{\sqrt{A - \cos \phi}} \, d\phi$$  \hspace{1cm} (6.46)
which can be integrated in terms of elliptic integrals to obtain
\[
y = \sqrt{2} \left( \frac{A}{\sqrt{A-1}} F\left( \frac{\phi}{2} | \frac{A-1}{A-1} \right) - \sqrt{A-1} E\left( \frac{\phi}{2} | \frac{A-1}{A-1} \right) \right)
\]
(6.47)

It remains to determine \( A \). Since \( \eta(W) = \sqrt{2} A \), \( A \) must satisfy
\[
W = \int_0^{\pi/2} \frac{\cos \phi}{\sqrt{A - \cos \phi}} \, d\phi
\]
(6.48)

This defines \( A \), but cannot be solved to give \( A \) in terms of known functions. A graph of \( A \) as a function of \( W \) is shown in Figure 6.13.

Figure 6.13: The constant \( A \) as a function of channel width \( W \).

6.3.1 Boundary Tracing Equation (6.44) gives \( \eta_v \) as a function of \( \eta \)
\[
\frac{d\eta}{dy} = \frac{\sqrt{1 - (A - \eta^2/2)^2}}{A - \eta^2/2}
\]
(6.49)

Now the boundary condition is
\[
\nabla \eta \cdot \hat{n} = F = \cos \gamma \sqrt{1 + \eta_v^2} = \frac{\cos \gamma}{A - \eta^2/2} = G(\eta)
\]
(6.50)

Since \( \eta_v \) and \( F \) can be expressed in terms of \( \eta \) we can use the results of Subsection 3.5.3.
\[
x = C \pm \int \frac{G}{\eta_v \sqrt{\eta_v^2 - G^2}} \, d\eta
\]
(6.51)
\[
= C \pm \cos \gamma \int \frac{A - \eta^2/2}{\sqrt{1 - (A - \eta^2/2)^2} \sqrt{\sin^2 \gamma - (A - \eta^2/2)^2}} \, d\eta
\]
(6.52)
\[
= C \pm \cos \gamma \int \frac{\cos \phi}{\sqrt{A - \cos \phi \sqrt{\sin^2 \gamma - \cos^2 \phi}}} \, d\phi
\]
(6.53)

which unfortunately cannot be integrated in terms of known functions.
6.3.2 Corner Results We can calculate the height, $H$, in a corner created by piecing together two of these traced boundaries. The easiest way of doing this is using (3.4)

$$\sin \alpha = \frac{F}{\|\nabla \eta\|}$$

This gives

$$\sin \alpha = \frac{\cos \gamma}{\sqrt{1 - \left(A - \eta^2/2\right)^2}}$$

(6.55)

Solving this for $\eta$ and substituting $k = \sin \alpha / \cos \gamma$ we obtain

$$H = \sqrt{2} \sqrt{A - \sqrt{1 - k^{-2}}}$$

(6.56)

Clearly $A$ represents the influence of the far wall on the local behaviour. When $A = 1$ this equation reduces to the half-plane case.

6.4 Micro-scale Roughness

The measured length for the perimeter of an object depends upon how closely we approximate the geometry. For example, real surfaces have tiny dents, cracks and imperfections all of which may affect the measured length of the perimeter. Consideration of such small scale geometry can lead to an understanding of macroscopic properties.

This idea is not new; studies of lighting for computer graphics, such as those by Oren and Nayar [27], have used very small geometry or micro-facets to obtain macroscopic lighting properties.

Here we look at the effects of very small scale geometry with a contact angle $\gamma$ on the effective macroscopic contact angle $\gamma$. This will be done by constructing a variety of simple rough surfaces with exact solutions and observing what effect introducing microscale roughness has on solution behaviour.

In the area of computer graphics microscale techniques typically use stochastic techniques rather than using regular exact solutions. It is suggested by Oren and Nayar [27] that this is necessary as a regular model can introduce bias. In these lighting simulations non-linearity does not cause the serious technical difficulties that it can cause for other non-linear PDEs. Thus we may expect that the bias introduced through the use of these regular rough surfaces may be more extreme for the Laplace-Young equation than lighting simulations$^4$.

$^4$The techniques of this chapter can easily be generalised to stochastic methods using irregular rough surfaces with random variation of the local values of $\cos \gamma$ and geometry. These generalisations produce the same results as those presented here.
These results are based on local approximation to the original boundary. First we will look at exact results obtained using boundary tracing in the half-plane, then extend these to more general geometry.

Using the divergence structure of the Laplace-Young equation it will be shown that if there is an effective contact angle, it must be the value derived here.

Finally numerical calculations show that these effective boundary conditions are applicable to other, non-boundary traced, rough surfaces.

6.4.1 What is Roughness? Let $L$ be the length of a curve $C$ when measured at some macroscopic length scale, while at some smaller, microscopic, length-scale the length of $C$ is $\bar{L}$. The roughness of the curve is defined to be $\rho = \frac{\bar{L}}{L}$. Evidently the definition of roughness depends upon the choice of the two scales.

6.4.2 Simple Line From the one dimensional solution to the Laplace-Young equation it is possible to construct an arbitrarily small single “tooth” from two pieces of traced boundary with $\nabla \eta \cdot \hat{n} = \cos \gamma$. Joining such teeth together produces a boundary which is a straight line at a large scale, but resembles a saw edge at a smaller scale. Such boundaries are shown in Figure 6.14 on this page. At the microscopic scale the boundary satisfies $\nabla \eta \cdot \hat{n} = \cos \gamma$ while at the macroscopic scale it satisfies $\nabla \eta \cdot \hat{n} = \cos \gamma$ for some $\gamma$.

![Figure 6.14: A top view of rough surfaces generated with two different teeth sizes.](image)

For the toothed surface let $\theta$ be the angle between the normal, $\hat{n}_t$, and $\nabla \eta$. Then

$$\frac{\nabla \eta \cdot \hat{n}_t}{\sqrt{1 + (\nabla \eta)^2}} = \frac{\|\nabla \eta\| \cos \theta}{\sqrt{1 + (\nabla \eta)^2}} = \cos \gamma$$  \hspace{1cm} (6.57)

For the straight line $\hat{n}$ is parallel to $\nabla \eta$ so

$$\frac{\|\nabla \eta\|}{\sqrt{1 + (\nabla \eta)^2}} = \cos \gamma$$  \hspace{1cm} (6.58)
6.4. Micro-scale Roughness

Thus \( \cos \theta = \frac{\cos \gamma}{\cos \tilde{\gamma}} \)

The roughness, \( \rho \), of this curve is the ratio of the length of the “toothed” surface, \( \bar{L} \), to the length of the line segment it approximates, \( L \). Simple geometry gives \( \rho = \frac{\bar{L}}{L} = \frac{1}{\cos \theta} \).

Finally the relationship

\[
\mu = \frac{\cos \tilde{\gamma}}{\cos \gamma}
\]

(6.59)

between the roughness of the surface, the real (microscopic) contact angle \( \gamma \) and the effective contact angle \( \tilde{\gamma} \) is obtained.

6.4.3 General Geometry Assume that locally the small scale solution behaviour is planar, \( \eta = Ax + b \). Let \( y = mx + c \) be the equation of the approximate “macroscopic” boundary between \( y_0 \) and \( y_1 \), satisfying \( \nabla \eta \cdot \hat{n} = \cos \gamma \). This section of boundary can be approximated arbitrarily well by “microscopic” line segments, each a tangent to traced boundaries, satisfying the same boundary condition with a different contact angle, \( \tilde{\gamma} \) see Figure 6.15. These segments have the form \( y = \pm \tilde{m}x + c_i \). On the line

\[
\frac{\nabla \eta \cdot \hat{n}}{\sqrt{1 + |\nabla \eta|^2}} = \frac{A}{\sqrt{1 + A^2 \sqrt{1 + m^2}}} = \cos \gamma
\]

(6.60)

On the microscopic approximation to this curve

\[
\frac{\nabla \eta \cdot \hat{n}}{\sqrt{1 + |\nabla \eta|^2}} = \frac{A}{\sqrt{1 + A^2 \sqrt{1 + \tilde{m}^2}}} = \cos \tilde{\gamma}
\]

(6.61)

Figure 6.15: Microscopic geometry of the form \( y = \pm \tilde{m}x + c_i \) (line) approximating macroscopic geometry (dotted line) of the form \( y = mx + c \).
The length of the macroscopic line is given by $(y_1 - y_0)\sqrt{1 + m^2}$ and the length of the microscopic approximation is given by $(y_1 - y_0)\sqrt{1 + \tilde{m}^2}$, so the ratio of their lengths is $\mu = \sqrt{1 + m^2}/\sqrt{1 + \tilde{m}^2}$.

Equations (6.60) and (6.61) show that the ratio of $\cos \gamma$ to $\cos \tilde{\gamma}$ is also given by $\sqrt{1 + m^2}/\sqrt{1 + \tilde{m}^2}$. This shows that the ratio of the "macroscopic" length of the boundary to the "microscopic" length of the boundary is also the ratio of the cosine of the "macroscopic" contact angle to the cosine of the "microscopic" contact angle. Written in terms of the roughness $\mu$, we obtain

$$\mu = \frac{L}{\tilde{L}} = \frac{\cos \tilde{\gamma}}{\cos \gamma}. \quad (6.62)$$

This is the same value as was obtained earlier for the one-dimensional case (6.59).

6.4.4 Global Considerations Let $\Omega$ be the "macroscopic" domain and $\tilde{\Omega}$ be the corresponding domain containing the "microscopic" details. Using the divergence structure of the Laplace-Young equation and the boundary conditions we can obtain values for the volume of fluid raised by the two domains.

$$\int_{\Omega} \eta \, dA = \frac{1}{\kappa} \int_{\Omega} \nabla \cdot \frac{\nabla \eta}{\sqrt{1 + |\nabla \eta|^2}} \, dA \quad (6.63)$$

$$= \frac{1}{\kappa} \int_{\partial \Omega} \nabla \cdot \hat{n} \, d\Gamma \quad (6.64)$$

$$= \frac{|\partial \Omega| \cos \gamma}{\kappa} \quad (6.65)$$

Similarly

$$\int_{\tilde{\Omega}} \eta \, dA = \frac{|\partial \tilde{\Omega}| \cos \tilde{\gamma}}{\kappa} \quad (6.66)$$

Thus, for the volumes raised to be the same, it is necessary that

$$\mu = \frac{|\partial \tilde{\Omega}|}{|\partial \Omega|} = \frac{\cos \tilde{\gamma}}{\cos \gamma} \quad (6.67)$$

Again we obtain (6.59), the roughness is the ratio of the cosines of the contact angles. This suggests that the roughness as defined can be used to provide the effective boundary condition

$$\frac{\nabla \eta \cdot \hat{n}}{\sqrt{1 + (\nabla \eta)^2}} = \rho \cos \tilde{\gamma} \quad (6.68)$$

in a variety of cases.

This can be observed numerically.
6.4.5 Numerical Examples  Here the Laplace–Young equation is solved in semi-infinite domains of the form

\[ y > A \cos \frac{\lambda x}{2\pi} \]  \hspace{1cm} (6.69)

using a non-linear finite element technique using linear triangular elements. A typical mesh is shown in Figure 6.16. For each case the roughness coefficient (compared with a straight line) was calculated. Selected results are shown in Figure 6.17.

Figure 6.16: A typical mesh used for calculating solutions to the Laplace–Young equation in realistic domains.

It can be seen that the rough approximation is a reasonable fit, especially for the smaller amplitude cases. The approximation for \( A = 0.2, \lambda = 0.1 \) is still a much better approximation than replacing the rough wall with a smooth wall with the same contact angle. These results are shown in Figure 6.18, with the numerical solution, the rough-wall approximation and the solutions for a wall at \( y = 0 \), \( y = -A \) and \( y = +A \).

These results suggest that the rough boundary results are applicable to a wide variety of situations and not just those generated by piecing together traced solutions.

6.5 Radial Tracing

Tracing a boundary numerically is relatively easy when \( \eta \) is known exactly but the radially symmetric solutions to the Laplace–Young equation are only known asymptotically. Consequently we have to resort to numerical techniques.
6.5.1 The Behaviour of the $\eta(r)$ Solutions In the earlier sections we noted that the solution to the half plane problem with specified boundary conditions could be extended past the boundary, giving a general solution for any contact angle. This extension is to a finite distance only and at its furthest point there was a singularity in the surface behaviour.

It is not surprising that a similar situation occurs for the solution in a cylinder. We are only able to extend the solution in a cylinder of radius $R$ out to a singularity a distance $R_\ast$ from the origin. From this extended solution we can find solutions in cylinders with various combinations of $r$ and $\gamma$. As $r$ approaches zero, $\gamma$ approaches zero and as $r$ approaches $R_\ast$, $\gamma$ approaches $\pi/2$.

A similar situation occurs for annular domains where the solution in the annulus $r_1 < r < r_2$ can only be extended to another annulus $r_1^* < r < r_2^* < r_2$ with singularities at $r = r_1^*$ and $r = r_2^*$. This behaviour can be seen in Figure 6.19.

6.5.2 The Numerical Technique The function $\eta(r)$ can be found using numerical integration. The boundary tracing problem could then be solved numerically using this approximation. However this introduces problems as the sample points from the calculation of $\eta$ do not necessarily match up with the points needed to
6.5. Radial Tracing

### Approximate and Numeric solutions in y>0.2 cos(0.1 x/(2 PI» with cos(\gamma_H»*<3 PI/7)

- **Numerical Solution**
- **Approximate Solution**
- **Half Plane solution in y>0.2**
- **Half Plane solution in y<0.2**

Figure 6.18: The numerical solution in a rough domain compared with the rough approximation and solutions obtained by replacing the mean, maximum and minimum boundary positions with a straight wall with equivalent boundary conditions.

We can calculate the boundary. Moreover we would expect to find \( \eta \) as a function of \( r \) and the boundary as a function of \( \theta \). These difficulties lead to an unacceptable amount of error for reasonable step sizes.

Instead a combined approach was used where the solutions for \( \eta(r) \) and \( r(\theta) \) are derived simultaneously. This is done using a system of three first order nonlinear ODEs.

Letting \( \eta = g(r) \) and the boundary be \( r(\theta) \), the boundary condition becomes

\[
\frac{rg'(r)}{\sqrt{1+g'^2} \sqrt{r^2 + (r')^2}} = C
\]

(6.70)

The PDE becomes

\[
g' + (g')^3 + rg'' = g
\]

(6.71)

Letting \( y_1 = \eta = g \), \( y_2 = \eta_r = g' \) and \( y_3 = r(\theta) \) we obtain

\[
\dot{y}_1 = \frac{d\eta}{dr} \frac{dr}{d\theta} = y_2 \dot{y}_3
\]

(6.72)

\[
\dot{y}_2 = \frac{d\eta_r}{dr} \frac{dr}{d\theta} = \frac{1 + y_2^2}{y_3} \left(-y_2 + y_1 y_3 \sqrt{1 + y_2^2}\right) \dot{y}_3
\]

(6.73)

\[
\dot{y}_3 = \frac{dr}{d\theta} = \frac{y_3 \sqrt{(1 - c^2)y_2^2 - c^2}}{c \sqrt{1 + y_2^2}}
\]

(6.74)
These were solved using a fourth-order Runge-Kutta method, giving the solution in an annular domain.

The initial boundary conditions to be used were found by using a shooting method on the radial Laplace–Young to find the values of $y_i$ on the inner and outer boundaries, $r_i$ and $r_o$. The region between $r_i$ and $r_o$ is the non-viable region. The values of $\eta(r_i)$ and $\eta_r(r_i)$ were then used to obtain appropriate starting values inside the viable domain for the numerical scheme (6.72).

Typical domains that can be obtained from the solution in an annulus can be seen in Figure 6.20 (See Figure C.12 for colour version). In a similar manner solutions in rough cylinders can be constructed.
6.6 Conclusion

A key result of this chapter was the discovery of a large family of new exact domains with corners in which the Laplace–Young equation has analytic solutions. These domains provided analytic examples of a range of known asymptotic behaviour as well as new results concerning corner height.

New results for rough boundaries were also developed. The domains were produced by small-scale boundary tracing, with the results being supported both numerically and through energy arguments.

These two sets of results show that boundary tracing can provide new information about solution behaviour for difficult non-linear PDEs.
CHAPTER 7

Rounded Corners

7.1 Introduction

Boundary tracing can be used to investigate the effect of corner rounding on the behaviour of solutions to Helmholtz's and the Laplace–Young equations.

The Laplace–Young equation is considered because interesting behaviour is known to occur near sharp corners as was mentioned in Chapter 6. Helmholtz's equation is used as an approximation to the Laplace–Young equation.

7.1.1 Chapter Overview Initial investigations on Helmholtz's equation show that the solution in a wedge admits a smooth, symmetric traced boundary curve. However this single curve does not provide much useful information about the interplay of smoothing and height-rise. A method for generating traced boundaries with a variety of smoothed corners is obtained through superposition.

A relationship between corner rounding and corner height rise is obtained for the domains generated. This relationship provides a useful approximation for a variety of situations with smoothed corners.

The relationship obtained suggests that, in general, small scale rounding lowers the solution while large scale rounding raises the solution. A proof of this is presented in Subsection 7.2.6 with the large scale rounding case requiring slight modifications to the boundary.

Clearly the methods involving superposition fail for the nonlinear Laplace–Young equation, so that the families of symmetric smooth boundaries cannot be obtained by boundary tracing. However, the results concerning the global effects of corner rounding carry over relatively simply.

7.1.2 What Does Corner Rounding Mean? Intuitively rounding a corner involves replacing a sharp corner with a smoothed corner.

The principle characteristics of corner rounding are that the new curve must behave like the original curve away from the corner and have non-zero radius of curvature near the corner. Also the new boundary should be entirely concave or convex near the vertex. Clearly there is more than one way to smooth any given corner.

Since there is no obvious universal measure for determining whether one curve is a rounded version of another, this decision is subjective. However, the minimum radius of curvature of the rounded corner provides a useful way to quantify the amount of rounding.
Chapter 7. Rounded Corners

The results obtained here are primarily for symmetric rounded wedge domains.

7.1.3 Why is rounding interesting? The rounding of corners is of interest physically as most real-world corners are rounded at some small scale. Whether this rounding affects the global behaviour of the solution depends to a significant degree upon the nature of the PDE. In particular, it is well known that for an elliptic PDE the boundary conditions/geometry can influence the solution behaviour everywhere in the domain.

For numerical or analytic purposes it is easier to use sharp corners than corners rounded at some small scale. The influence this has on solution behaviour can be better understood through examining the potential effects of corner rounding.

Corner rounding is particularly important for the Laplace—Young equation, where sharp corners can have drastic effects on solution behaviours, such as the introduction of infinite solution height or discontinuities, as was discussed in Chapter 6.

7.2 Helmholtz’s equation

7.2.1 A Simple Example Helmholtz’s equation with the boundary conditions \( \nabla \eta \cdot \hat{n} = 1 \) has the simple solution \( \eta = e^{-x} + e^{-y} \) in the quarter plane \( x > 0, \ y > 0 \). If this solution is used as a base function for finding traced boundaries then the curves shown in Figure 7.1 are obtained. Of particular interest are the two traced boundaries having the same axis of symmetry as the original domain, shown in Figure 7.2.

It is possible to calculate the position of the tip of these smooth symmetric curves and their curvature at this point. By symmetry the tip is on the line \( y = x \) and must have \( \eta_x = \eta_y = -1/\sqrt{2} \). This occurs at

\[
x = y = \frac{\ln 2}{2}
\]

The height of the solution at the tip, \( H \), is given by

\[
H = \sqrt{2}
\]

Considering the boundary and gradient directions it is obvious that at the tip the gradient of \( \eta \) and tangent to the rounded corner will be perpendicular (i.e. \( \nabla \eta \cdot \hat{r} = 0 \)) thus the tip lies on the terminal curve. In fact it is a critical terminal point. Since there are two curves through the tip it must be a saddle type point and the two smooth curves are the separatrices of the saddle. This can be seen on the manifold in Figure 7.3 and can be verified easily:
Section 3.3 demonstrated that the behaviour of the traced boundaries at a terminal critical point depended upon the value of \((\kappa_\Phi - \kappa_\eta)\), where \(\kappa_\Phi\) and \(\kappa_\eta\) are the curvatures of the contours of \(\Phi\) and \(\eta\) respectively.

Now \(\Phi\) is given by

\[
\Phi = \|\nabla \eta\|^2 - 1 = e^{-2x} + e^{-2y} - 1
\]  

so we can see that at the tip \(\nabla \Phi_0 = -[1]\) while \(\nabla \eta = -\frac{1}{\sqrt{2}}[1]\). Thus \(\lambda = \frac{1}{\sqrt{2}}\).

The curvatures \(\kappa_\eta\) and \(\kappa_\Phi\) can be calculated giving

\[
\kappa_\eta = \frac{(Q\nabla \eta)^T H(Q\nabla \eta)}{\|\nabla \eta\|^3} \quad \kappa_\Phi = \frac{(Q\nabla \Phi_0)^T H_\Phi(Q\nabla \Phi_0)}{\|\nabla \Phi_0\|^3} \quad (7.4)
\]
\[
= \frac{(-1/\sqrt{2}[1])^T (1/\sqrt{2} I) (-1/\sqrt{2}[1])}{\|1/\sqrt{2} [1]\|} = \frac{1}{\sqrt{2}} \quad (7.5)
\]
\[
= \frac{2}{\sqrt{2}} \quad (7.6)
\]

Thus \((\kappa_\Phi - \kappa_\eta) = \frac{1}{\sqrt{2}} > 0\) so the critical point must be a saddle point on the manifold and as we have already seen, there will be two smooth curves through the point.

Similarly using the formula for the curvature at a critical terminal point, (3.36), the curvature at the tip of the traced boundaries can be found to be the roots of

\[
\kappa^2 + \kappa/\sqrt{2} - 1/2 = 0 \quad (7.7)
\]
Figure 7.2: There are two symmetric traced solutions and both are tangential to the terminal curve (not shown) at the same point. Only one remains within the quarter plane.

i.e. \( \kappa \approx 0.437016 \) or \( \kappa \approx -1.14412 \). Thus there is a rounded wedge with half angle \( \alpha = \pi/4 \) and radius of rounding \( r \approx (1.14412)^{-1} \approx 0.874 \), having the same solution as the quarter plane and height at the tip of \( H = \sqrt{2} \).

7.2.2 Other Angles The earlier example contained nothing that was specific to the 90-degree wedge. Since exact solutions in wedges of any angle have been derived by Fowkes and Hood [11] these solutions can, in principle, be used to obtain traced boundaries. However, due to the complexity of the base functions, tracing boundaries becomes difficult for all except those solutions expressible using the method of images. The traced boundaries for several of these cases are shown in Figure 7.4. Note that in each of these cases the existence of a saddle type terminal critical point, with associated smooth symmetric boundaries, is evident.

7.2.3 Other Radii To understand the effect of rounding on solution behaviour it is not enough to have a single isolated example.

Solutions for arbitrary wedge angles can be derived but each angle provides only one symmetric traced boundary and consequently only one radius of rounding. We would like to be able to vary the radius of rounding for fixed \( \alpha \). To do this a range of base functions must be available for each wedge angle. Because of Helmholtz’s equation’s linearity this can be done easily, either through scaling\(^1\) or by the addition

\(^1\)Using boundary tracing on the scaled wedge solution \( \tilde{\eta} = A\eta \) gives new symmetric boundary curves offset from the original wedge domain. Unfortunately this method fails for the quarter...
7.2. Helmholtz's equation

Figure 7.3: Three views of the boundary curves on a manifold for Helmholtz's equation in a corner. Left: Top view. Center: View along $x = y$. Right: Three Dimensional view.

Figure 7.4: Views of boundaries, on their associated manifold, traced in wedges with angles $\alpha = \pi/6$ and $\alpha = \pi/8$.

of a source like term. Only the addition of source terms will be considered here.

The separated solutions to Helmholtz's equation in radial coordinates with exponential decay as $r \to \infty$ are

$$\mu = K_r(r) \cos(\lambda \theta + \phi)$$

(7.9)

Imposing symmetry about $\theta = 0$ and the additional constraint that the solution has plane, as

$$A \eta(x, y) = A(e^{-x} + e^{-y}) = e^{-(x - \ln(A))} + e^{-(y - \ln(A))} = \eta(x - \ln A, y - \ln A)$$

(7.8)

In this case the offset curves are simply translated copies of the original curve. This does not occur for other wedge angles.
\[ \nabla \mu \cdot \hat{n} = 0 \] on the wedge boundary gives

\[ \mu_n = K_{\lambda_n}(r) \cos(\lambda_n \theta) \quad (7.10) \]

where \( \lambda_n = \frac{(2n+1)\alpha}{2\alpha} \). Consider a function, \( \tilde{\eta} \), of the form

\[ \tilde{\eta} = \eta_W + \sum_{i=0}^{N} \epsilon_i K_{\lambda_n}(r) \cos(\lambda_n \theta) \quad (7.11) \]

where \( \eta_W \) is the normal wedge solution in the wedge of half angle \( \alpha \) symmetric about \( \theta = 0 \). Clearly \( \tilde{\eta} \) solves Helmholtz's equation in the wedge, with \( \nabla \tilde{\eta} \cdot \hat{n} = 1 \) on the edge of the wedge \( \theta = \pm \alpha \). These solutions have a singularity at the origin. This singularity is not a problem as it will be outside the traced domains.

Each choice of the \( \epsilon_i \)'s leads to a new solution and each of these solutions provides 0, 1 or 2 new smooth boundaries, depending on the nature of the terminal critical point. Whilst the available number of solutions has been increased dramatically only cases of the form

\[ \tilde{\eta} = \eta_W + \epsilon K_0(r) \quad (7.12) \]

where \( \epsilon_0 = \epsilon \), will be considered. Other solutions with non-zero higher terms, \( \epsilon_i \neq 0 \) for \( i > 0 \), tend to have badly behaved traced boundaries if the \( \epsilon_i \) are chosen arbitrarily\(^2\).

### 7.2.4 A Formula Relating \( r \), \( \alpha \) and \( H \)

Since each choice of \( \epsilon_0 = \epsilon \) leads to a new base function, the height and radius of rounding can be calculated for a variety of cases. In fact all the necessary information about local behaviour can be calculated using the values of \( \eta \) and \( K_0 \) along the center of the wedge.

Let \( p \) be a point on the axis of symmetry and \( \hat{s} \) be the unit vector along the line of symmetry so that \( p = R\hat{s} \) for some \( R \). Define \( f(r) = \eta(r\hat{s}) \) and \( g(r) = K_0(r) \). Then the height along the center line of a wedge solution of the form (7.12) is given by

\[ h(r) = f(r) + \epsilon g(r) \]

\(^2\)It is possible to use Fourier-like methods with these functions to impose the boundary condition \( \nabla \eta \cdot \hat{n} \approx 1 \) on a given rounded corner curve. That is, given the boundary \( \partial \Omega \) finding \( \epsilon_i \)'s such that

\[ \int_{\partial \Omega} (\nabla \tilde{\eta} \cdot \hat{n} - 1)^2 \, ds \quad (7.13) \]

is minimised, where \( \tilde{\eta} \) is given by (7.11), should give a good approximation to the solution. Unfortunately this method is numerically unstable.
We can find $\epsilon$ such that there may exist a traced boundary curve through $p$ which is smooth, symmetric and satisfies $\nabla \bar{\eta} \cdot \bar{n} = 1$. This occurs when

$$f'(R) + \epsilon g'(R) = -1$$

giving $\epsilon$ as a function of $R$

$$\epsilon = -\frac{1 + f'(R)}{g'(R)} \quad (7.14)$$

Assuming that boundary tracing from the point $p$ produces a well behaved smoothing of the wedge, we are interested in the height of $\eta$ and curvature of the boundary curve at the point $p$.

Clearly the height at $p$ is

$$H(R) = f(R) + \epsilon(R)g(R) \quad (7.15)$$

Since $p$ is a critical terminal point the curvature at $p$ is given by $(3.34)$. As $\bar{\eta}$ is a solution to Helmholtz's equation and due to the symmetry of the domain, the derivatives of $\bar{\eta}$ can be expressed using $f$, $g$ and $\epsilon$. Substituting these derivatives into $(3.34)$ gives the following quadratic for $\kappa$.

$$\kappa^2 + \kappa(3f'' - 2f + \epsilon(3g'' - 2g)) + ((f' - f'') + \epsilon(g' - g'')) = 0 \quad (7.16)$$

Letting $\Delta(R)$ be the discriminant of the quadratic

$$\Delta = ((3f'' - 2f) + \epsilon(3g'' - 2g))^2 + 4((f' - f'') + \epsilon(g' - g'')) \quad (7.17)$$

then for $\Delta \geq 0$ we obtain two curvatures given by

$$\kappa = \frac{-(3f'' - 2f) + \epsilon(3g'' - 2g)) \pm \sqrt{\Delta}}{2} \quad (7.18)$$

Whilst $(7.15)$ and $(7.18)$ seem to produce an implicit relationship between curvature and height, things are not that simple. There are several potential problems.

1. Some values of $p$ do not produce symmetric boundaries, as for $\Delta(R) < 0$ the terminal critical point is a spiral point rather than a saddle point, see Section 3.3.
2. Although the local behaviour of the traced boundaries is known, information about their "global behaviour" is not. Thus it is possible that the curves are not suitable roundings of the wedge domain. For example the traced boundary may hit the terminal curve, or move away from the edges of the wedge.
3. Another problem is that there may be multiple values of $\epsilon$ giving the same radius of rounding but different heights.

Some of these problems will be demonstrated for the right-angled wedge case.

**Example 17.** The solution in a right-angled wedge is $\eta = e^{-x} + e^{-y}$. Thus the forced solution is given by

$$\eta = e^{-x} + e^{-y} + \epsilon K_0(r) \quad (7.19)$$

Graphs of the symmetric traced boundaries, for a variety of $\epsilon$, are shown in Figure 7.5. It can be seen that only some of the traced boundaries near the origin behave like rounded wedges. The intermediate traced boundaries, shown in grey, hit the terminal curve. The furthest out boundaries all curve in the wrong direction. This suggests that there are three cases.

1. For small $r$ one of the two traced boundaries is an acceptable rounding of the wedge, the other curves the wrong way.
2. Intermediate $r$ results in no symmetric smooth boundaries.
3. For large $r$ two symmetric smooth boundaries can be found but both curve the wrong way to be considered rounded wedges.

The curves for small $r$ can be seen in Figure 7.6.
7.2. Helmholtz's equation

Figure 7.6: Traced symmetric boundaries for $\eta = e^{-x} + e^{-y} + \epsilon K_0(r)$ with $\nabla \eta \cdot \hat{n} = 1$ and various small $\epsilon$.

The curvature of these curves can be obtained using the values of $\eta$ along the center line. Using the earlier results of this section we obtain

$$f(r) = 2e^{-r/\sqrt{2}} \quad (7.20)$$
$$g(r) = K_0(r) \quad (7.21)$$
$$\epsilon(r) = \frac{1 - \sqrt{2}e^{-r\sqrt{2}}}{K_1(r)} \quad (7.22)$$

Similarly we can calculate $\Delta(r)$, the discriminant of the curvature polynomial. Graphs of $\epsilon(r)$ and $\Delta(r)$ can be seen in Figure 7.7.

Figure 7.7: $\epsilon(r)$ and $\Delta(r)$ for $\eta = e^{-x} + e^{-y} + \epsilon K_0(r)$.

It is clear that for some range of $r$ (calculated numerically to be $0.596 < r < 2.06$) $\Delta(r) < 0$. For these values of $r$ the terminal critical point is a spiral point and there are no symmetric traced boundaries through the point. For $r < 0.596$ rounded wedges are obtained. For $r > 2.06$ the traced boundaries curve the wrong direction.
The curvatures over the valid ranges of $r$ are shown in Figure 7.8. For small

![Curvature](image)

Figure 7.8: The two curvatures $\kappa_1$ and $\kappa_2$ of the boundaries through $p = r\delta$.

there are two choices for $\kappa$: one positive, one negative, the negative choice corresponds to the rounded wedges while the positive choice corresponds to the curves that curve the wrong way in Figure 7.6. For large $r$ both traced boundaries do not behave like rounded wedges.

A parametric plot relating height and curvature can now be constructed using $r$ as the running parameter. This is shown over a large range of $r$ in Figure 7.9. The curves in Figure 7.9 are discontinuous and multi-valued for some choices of $\kappa$. However, we are only interested in the negative values of $\kappa$ as these correspond to boundaries that are shaped like rounded versions of the wedge. This single curve is well behaved.

![Height and Curvature](image)

Figure 7.9: The height (vertical) and curvature (horizontal) at the tip of the smooth symmetric traced boundaries plotted as parametric functions of the position of the tip.
The radius of curvature–height relationship obtained can be compared with the height obtained numerically in domains with corner rounded by a quarter circles of various radii. Both results can be seen in Figure 7.10.

Figure 7.10: Comparison of the analytic relationship between corner height and radius of rounding for traced boundaries (smooth) and numerically calculated values for corners rounded using a quarter circle.

The two derived curves differ by up to 10%. This “error” is due to the domain boundaries being significantly different. The results also suggest that terms other than local curvature of a rounded corner affect height rise.

Further detail about the problems that arise can be found by examining the traced boundaries through points other than the critical point. These traced boundaries were calculated numerically for different values of $\varepsilon$ and are shown in Figure 7.11.

For small negative values of $\varepsilon$ a hole is generated in the viable domain, between the singularity at the origin and the outer terminal curve. There are two smooth symmetric traced boundaries that behave like rounded wedges. One comes from the terminal critical point at the end of the hole, the other from a critical terminal point on the other terminal curve.

The left-most figures in Figure 7.11 show the traced-boundary behaviour for $\varepsilon < 0$. The lower left image displays the behaviour of the curves on the manifold near the “outer” critical terminal point. The figure to the right shows the behaviour for the “inner” critical terminal point. Both cases are saddles so smooth traced boundaries exist through the points as seen earlier. The center images of Figure 7.11 show the behaviour for $\varepsilon = 0$, which has already been examined. The figures to the right of this are for larger values of $\varepsilon$.

---

3As $\varepsilon$ becomes more negative the two non-viable domains merge.
It is notable that there is the development of two additional saddle points on the manifold, on either side of the central point. Also the behaviour of the center saddle point changes to a spiral point \( (\epsilon = 5.5) \), then back to a saddle point for large \( \epsilon \) \( (\epsilon = 20.6) \). This is consistent with earlier observations. For large \( \epsilon \) the behaviour of traced boundaries far from wedge edges resembles that of the boundaries for the radial solution \( \epsilon K_0(r) \) alone. This is not surprising since \( 0 \approx \| \nabla \eta \| \ll \| \epsilon \nabla K_0(r) \| \).

Figure 7.11: Comparison of traced boundary behaviour for the “forced” solution in a wedge for different amounts of forcing. Shows top view of traced boundaries and view of boundaries on the associated manifold seen along the axis of symmetry.

This example produces a sensible relationship between \( \kappa \) and \( H \), however the relationship is only accurate over limited ranges of \( \kappa \). Also since different relationships could be derived by using different combinations of source terms, the height in a rounded corner cannot be determined purely by the local maximum curvature.

This is not surprising, as it has already been shown in Example 16 that in some situations far field geometry plays a significant role in the corner height for sharp corners. Presumably the same is true near rounded corners.

7.2.5 Some Observations Although the search for a functional relationship between height-rise, corner angle and radius of rounding was of limited success, the results obtained are enough to suggest an important general result. In particular, the small negative values of epsilon correspond to “small scale” rounding and positive values of epsilon correspond with “large scale” rounding. Here large and small scale is relative to symmetric boundary for the unperturbed \( (\epsilon = 0) \) base function.

Now since \( K_0(r) \) is strictly positive, the base function \( \bar{\eta} = \eta + \epsilon K_0(r) \) is less than \( \eta \) for \( \epsilon \) negative and greater than \( \eta \) for \( \epsilon \) positive. This suggests that the
unperturbed traced symmetric boundary is special: "tighter" corners result in a solution that is globally lower than the wedge solution and "looser" corners have globally higher solution. The unperturbed traced boundary is in between, leaving the solution unchanged.

### 7.2.6 The Effect Of Corner Rounding

The results of Subsection 7.2.5 can be made stronger using a known result concerning the effect of changed boundary conditions on solution height (a comparison theorem).

**Theorem 4.** Let $\Omega \subset \mathbb{R}^2$. If $\eta$ and $\bar{\eta}$ both solve Helmholtz's equation (5.1) in some domain $\Omega$ with the boundary conditions $\nabla \eta \cdot \hat{n} = f$ and $\nabla \bar{\eta} \cdot \hat{n} = g$ with $f \geq g$ at all points on $\partial \Omega$, then $\eta \geq \bar{\eta}$ everywhere in $\Omega$.

**Proof.** (Adapted from Protter & Weinberger [28])

Let $u = \eta - \bar{\eta}$ then
\[
\begin{align*}
\nabla^2 u - \kappa u &= 0 & \text{in } \Omega \\
\nabla u \cdot \hat{n} &= f - g \geq 0 & \text{on } \partial \Omega
\end{align*}
\]

Now the PDE cannot have a non-positive minimum (non-negative maximum) in $\Omega$. So any negative minima occur on $\partial \Omega$.

Assume that $u$ has a negative minimum at $\xi$ on $\partial \Omega$. Then by the Hopf Maximum Principle, the outward normal derivative $\nabla u(\xi) < 0$. This contradicts $\nabla u \cdot \hat{n} \geq 0$ on $\partial \Omega$.

Thus $u \geq 0$ on $\partial \Omega$ and hence also $u \geq 0$ on $\Omega$. Thus $\eta \geq \bar{\eta}$. □

Let $W$ denote a wedge domain and let $\eta_W$ be the solution to Helmholtz's equation with boundary condition $\nabla \eta \cdot \hat{n} = c$ on the edges of $W$. Consider a domain $S$ which is the same wedge domain with smoothed corner. Let the normal to $\partial S$ be $\hat{n}_S$ and the solution to Helmholtz's equation with boundary condition $\nabla \eta \cdot \hat{n} = c$ in $S$ be $\eta_S$. Theorem 4 can be used to compare $\eta_S$ with $\eta_W$ inside $S$.

If $\hat{n}_S \cdot \nabla \eta_W < \hat{n}_S \cdot \nabla \eta_S = c$ everywhere on $\partial S$ then $\eta_S > \eta_W$ inside $S$. Conversely $\eta_S < \eta_W$ if $\hat{n}_S \cdot \nabla \eta_W > c$.

Since $\nabla \eta_W$ is relatively large near the vertex of a wedge, $\nabla \eta_W \cdot \hat{n}_S \geq c$ on smooth boundaries near the vertex. Thus the corresponding domains will have globally lower solutions. Similarly $\nabla \eta_W$ will be small far from the vertex and boundaries, causing large scale rounding curves to have $\nabla \eta_W \cdot \hat{n}_S \leq c$. Consequently the corresponding domains will have lower solutions.

This can be seen by using the quarter plane and rounding the tip of the domain using quarter circles.
Example 18. Consider the quarter plane with tip rounded using quarter circles, as shown in Figure 7.12. The solution inside the wedge is \( \eta_W = e^{-x} + e^{-y} \). We denote the normal to the smoothed domains as \( \mathbf{n}_S \). Figure 7.13 shows \( \nabla \eta_W \cdot \mathbf{n}_S \) as a function of \( \theta \) along the edge of circular arcs, for varying radii. The upper curves are for small \( r \), the lower curves for larger \( r \).

![Figure 7.12: Quarter circles of various radii, rounding the corner of the quarter plane domain.](image)

Figure 7.13: \( \nabla \eta_W \cdot \mathbf{n}_S \) along a circular arcs for \( \eta_W = e^{-x} + e^{-y} \). The upper curves are for small \( r \) the lower curves for larger \( r \). The darker curve is \( r = 1.18 \).

It can be seen that there is some \( R_{\text{min}} \approx 1.18 \) such that for \( r < R_{\text{min}} \) the arcs have \( \nabla \eta_W \cdot \mathbf{n}_S \geq 1 \) for \( 0 \leq \theta \leq \pi/2 \). This defines small scale rounding. Similarly for large \( r \) the arcs have \( \nabla \eta_W \cdot \mathbf{n}_S < 1 \) over most of their length. Further analysis shows that for large \( R \) the region where \( \nabla \eta_W \cdot \mathbf{n}_S > 1 \) is of size \( e^{-R}/(R+1) \).
In this example, “small” rounding leads to a globally lower solution, \( \eta_s \leq \eta_w \) using Theorem 4.

Unfortunately we cannot conclude that “large” rounding leads to a globally higher solution as \( \nabla \eta_w \cdot \hat{n} \leq 1 \) is not true for all \( \theta \). We can get around this problem by replacing the part of the boundary having \( \nabla \eta_w \cdot \hat{n}_s > 1 \) with a piece of traced boundary with \( \nabla \eta \cdot \hat{n} = 1 \), resulting in a new domain \( \hat{S} \). This replacement will be smooth and for large enough \( R \) it will be only a minor change to the boundary. This new boundary has \( \nabla \eta_w \cdot \hat{n}_S \leq 1 \) for all \( \theta \), so the solution in the modified rounded domain will be globally higher, by Theorem 4. That is \( \eta_S \geq \eta_w \). Presumably the small modification will not change the solution much so that \( \eta_S \approx \eta_S \). Thus we expect \( \eta_S > \eta_w \) over most of the domain.

What can we say in the case where the rounding occurs very close to the vertex of the wedge? In this case \( \eta \) near the vertex is given by

\[
\eta_w = \frac{c \pi}{2 \kappa \alpha} - \frac{c \alpha}{\sin \alpha}
\]  

(7.23)

Then the gradient of \( \eta \) is locally like

\[
\nabla \eta_w = \frac{-c}{\sin \alpha} \hat{i}
\]  

(7.24)

Letting \( \hat{r} = (\cos \phi, \sin \phi) \) be the unit tangent to a curve \( C \) we see that if \( \alpha < |\phi| < \pi/2 \) at all points on the curve then \( \nabla \eta_w \cdot \hat{n}_s > c \). Geometrically this condition requires that the tangent line to the curve either crosses both edges of the wedge or is parallel to one of the edges. Theorem 4 implies that a boundary of this shape with the typical boundary conditions must lower the solution height everywhere.

Similarly if the tip of the smooth boundary is far from the origin it will be outside the viable domain, \( ||\nabla \eta_w|| < c \). Then since \( \nabla \eta_w \cdot \hat{n} < ||\nabla \eta_w|| \) a large part of the smooth boundary will have \( \nabla \eta_w \cdot \hat{n}_S < c \). It is only once this boundary crosses the terminal curve that this can become untrue. However when \( \nabla \eta_w \cdot \hat{n}_S = c \) we can smoothly replace the remaining (probably small) section of the curve with a traced curve, see Figure 7.14. This modified boundary has \( \nabla \eta_w \cdot \hat{n}_S \leq c \) everywhere and thus the corresponding modified domain has globally higher solution. Now if the modification was “small” we would expect the solution in the original domain to also be globally higher, except possibly near where the modification was required.

Small scale rounding of the wedge falls into the first category, causing globally lowered solution and large scale rounding of the tip gives the second case, resulting in a global or “nearly global” increase in solution height.
Chapter 7. Rounded Corners

Figure 7.14: The modified boundary with globally higher solution. The thick curve represents unchanged section of the original boundary. The thin black curve represents the section that has been replaced. The grey curve represents the traced replacement section. The terminal curve is shown dashed.

7.3 Laplace–Young

7.3.1 Complications As the Laplace–Young equation is not a linear equation and does not have known exact solution in a wedge it may seem impossible to extend the results of this chapter to the Laplace–Young equation.

Theoretically we could construct solutions to the Laplace–Young equation in a wedge (or almost wedge) domain numerically, then use numerical boundary tracing on these solutions. Practically this approach is limited as each solution leads to at most two symmetric traced boundaries that are rounded versions of the wedge. It would be as efficient and less complicated to construct rounded domains and solve the Laplace–Young equation in them directly. Fortunately this does not mean that there are no useful extensions to the Laplace–Young equation.

7.3.2 The Effect of Corner Rounding Although we cannot extend the use of the superposition methods to give us new rounded corners we can extend the global results. The Laplace–Young equation satisfies a similar condition to Theorem 4, The Maximum Principle of Concus and Finn [3, 8]

Theorem 5. Let $\Sigma = \Sigma^0 + \Sigma^a + \Sigma^b$ be a decomposition of $\Sigma$ (the boundary of $\Omega$) such that $\Sigma^b$ is either a null set of class $C(1)$ and $\Sigma^0$ is “small” in the sense introduced in §3.5 of [4]. Let $u$ and $v$ be of class $C(2)$ in $\Omega$ and suppose

4Typically there would only be at most one suitable boundary.

5Essentially that it is coverable by a sequence of sets of surfaces such that the sum of their area tends toward zero.
7.4. Conclusion

1. \( \nabla \cdot \frac{\nabla u}{\sqrt{1+(\nabla u)^2}} \geq \nabla \cdot \frac{\nabla v}{\sqrt{1+(\nabla v)^2}} \)

2. for any approach to \( \Sigma^\alpha \) from within \( \Omega \), \( \limsup (u - v) \leq 0 \)

3. on \( \Sigma^\beta \), \( \frac{\nabla u \cdot \hat{n}}{\sqrt{1+(\nabla u)^2}} \leq \frac{\nabla v \cdot \hat{n}}{\sqrt{1+(\nabla v)^2}} \) almost everywhere as a limit from points of \( \Omega \)

then \( u(x) \leq v(x) \).

Using this theorem, results equivalent to those obtained in Subsection 7.2.6 can be derived.

In particular looking at the local behaviour near a corner of angle \( \alpha < \pi/2 \) (see Subsection 6.1.2) again there is a region where \( \|\nabla \eta_W\| \) is large enough that we can construct curved boundaries with \( \frac{\nabla \eta_W \cdot \hat{n}}{\sqrt{1+\nabla \eta_W^2}} \geq c \), resulting in a corresponding domain with globally lower solution.

Fowkes and Hood [11] have suggested that far from the corner \( \eta_W \) behaves like the solution to Helmholtz's equation in the wedge. If this is the case then again rounded curves in the non-viable domain of the wedge solution which approach the boundary asymptotically will have globally higher solution. This means that slight (or no) modification of curves with large scale rounding gives curves with \( \frac{\nabla \eta_W \cdot \hat{n}}{\sqrt{1+\nabla \eta_W^2}} \leq c \), and the corresponding (possibly modified) domain has globally higher solution. This suggests that the original domain also had globally higher solution (except possibly near the modified boundary).

These results can be supported numerically. The solutions in a right angled wedge and several corresponding rounded domains were calculated numerically. The solution values along the center of the wedge are shown in Figure 7.15. The heights for the wedge with small scale rounding can be seen to be lower than those of the original wedge. Conversely the solution for the wedge with large scale rounding is higher.

7.4 Conclusion

Boundary tracing solutions to Helmholtz's equation in a wedge shows the existence of rounded domains with "simple" solutions. The existence of these curves was made evident using the manifold results of Chapter 3. The analytic height - curvature relationship obtained for these solutions was seen to provide a good approximation to the results obtained numerically in other rounded domains over a certain range of curvatures.

The solution behaviour for large and small scale rounding suggests the more general result that small scale rounding produces a globally lower solution whereas
large scale rounding produces a globally higher solution. The smooth traced boundaries play a dividing role, leaving the solution unchanged. The boundary tracing results could not be applied to the Laplace–Young equation due to its non-linearity. However the results pertaining to the global effects of corner rounding transferred to the Laplace–Young equation.

A variety of new results for Laplace–Young and Helmholtz's equations have been developed here. The techniques used to derive them have demonstrated that the increased flexibility available to linear PDEs allows some freedom in modifying boundary geometry. This chapter has also shown that boundary tracing can provide insight into complicated physical problems.

Figure 7.15: A comparison of the centerline height of numerical solutions in a right-angled wedge and two rounded versions.
Higher Order and Higher Dimensional Equations

In this chapter we investigate boundary tracing in higher dimensions and with higher order PDEs. In higher dimensions \( n \geq 3 \) boundary tracing is governed by first order PDEs rather than ODEs. There is correspondingly greater flexibility in the construction of the \( n \)-surfaces satisfying a given boundary condition than for curves in two dimensions. In contrast, higher order PDEs typically have more than one boundary condition imposed, further limiting boundary tracing. However, we will see that the flexibility available in higher dimensions can counteract the reduction in flexibility due to the extra boundary conditions of higher order PDEs.

8.1 Three dimensions

Here we consider the boundary condition

\[
\nabla \eta \cdot \hat{n} = F
\]

(8.1)

Where \( \eta : \mathbb{R}^3 \rightarrow \mathbb{R} \) is a prescribed base function, and \( \hat{n} \) is the normal to the required boundary surface in \( \mathbb{R}^3 \). Then as in (3.5) the angle \( \theta \) between the normal and \( \nabla \eta \) satisfies

\[
\cos \theta = \frac{F}{\|\nabla \eta\|}
\]

(8.2)

The functions \( F \) and \( \eta \) determine a unique value of \( \theta \) between 0 and \( \pi \). Recall that in two dimensions this gave two directions for the normals. In three dimensions an infinite number of directions are available. A geometrical interpretation is that the possible normals form a cone, which we will call viable cone, with axis \( \nabla \eta \) and opening angle \( \theta \). See Figure 8.1. Through each point there is an infinite number of surfaces satisfying the boundary condition. This can be seen in the symmetric cases.

In three dimensions there are many possible symmetries to examine. Only planar symmetry and spherical symmetry will be considered here.

In both cases the boundary tracing PDE can be solved to give an infinite family of boundary surfaces. This is achieved by obtaining complete integrals from which general integrals and singular integrals can be derived.\(^1\)

\(^1\)The definitions of complete, singular and general integrals of first order PDEs can be found in Murray's book [25] or most other classical PDE books.
Figure 8.1: The directions (if any) that are possible for normals satisfying $\nabla \eta \cdot \hat{n} = F$ form a cone about $\nabla \eta$, called the viable cone. The large arrow represents $\nabla \eta$ and the smaller, a normal in the viable cone.

8.1.1 Planar Symmetry Assuming that the base function, $\eta$, is of the form

$$\eta = f(z)$$

and the boundary condition, $\nabla \eta \cdot \hat{n} = F$ is of the form

$$\nabla \eta \cdot \hat{n} = F(\eta, \eta_z, z) = F(z)$$

then the problem has planar symmetry. Both $\eta$ and the boundary conditions are invariant under translation in the $x$ and $y$ directions.

In this case the gradient is given by

$$\nabla \eta = \begin{bmatrix} 0 \\ 0 \\ f'(x) \end{bmatrix}$$

Assuming that the boundary surface we are looking for is of the form

$$z = z(x, y)$$

Then its unit normal is given by

$$\hat{n} = \frac{1}{\sqrt{1 + z_x^2 + z_y^2}} \begin{bmatrix} -z_x \\ -z_y \\ 1 \end{bmatrix}$$

Clearly planar surfaces where $f'(z) = \pm F(z)$ satisfy the boundary conditions. However, other boundaries can also be obtained. The boundary condition can be written as

$$\nabla \eta \cdot \hat{n} = \frac{f'(z)}{\sqrt{1 + z_x^2 + z_y^2}} = F(g) \quad (8.3)$$
8.1. Three dimensions

It is possible to solve this first order PDE in general. The equation can be written as

\[ z_x^2 + z_y^2 = f'(z)^2/F(z)^2 - 1 \]  

(8.4)

where \( f'(z)^2/F(z)^2 - 1 \) is a known function of \( z \). Looking for a change of variables of the form \( U = h(z) \) for some \( h(z) \) leads us to

\[
\begin{align*}
U_x &= h'(z)z_x \\
U_y &= h'(z)z_y \\
U_x^2 + U_y^2 &= h'(z)^2(z_x^2 + z_y^2) \\
&= h'(z)^2(f'(z)^2/F(z)^2 - 1)
\end{align*}
\]

(8.5) \hspace{1cm} (8.6) \hspace{1cm} (8.7) \hspace{1cm} (8.8)

using (8.4). Thus choosing

\[ h(z) = \int \frac{dz}{\sqrt{f'(z)^2/F(z)^2 - 1}} \]  

(8.9)

equation (8.8) becomes the Eikonal equation

\[ U_x^2 + U_y^2 = 1 \]  

(8.10)

This PDE has known complete integrals which are just the planes

\[ U = \cos(\phi)x + \sin(\phi)y + A \]  

(8.11)

Thus a complete integral to (8.4) is the family of surfaces

\[ \cos(\phi)x + \sin(\phi)y + A = \int \frac{dz}{\sqrt{f'(z)^2/F(z)^2 - 1}} = h(z) \]  

(8.12)

Clearly this can only be integrated for \( |f'| > |F| \), which is the viable-region. The terminal surface is given by \( |f'| = |F| \) and is a valid boundary surface.

Note that this is similar to the result obtained in Section 3.5 for two dimensions when \( \eta = f(y) \) and \( \nabla \eta \cdot \hat{n} = F(y) \), \( x + C = \int (f'(y)^2/F(y)^2 - 1)^{-1/2} dy \).

Other smooth solutions are obtained by taking the envelope of a one parameter sub-family of these surfaces (general integrals) or the envelope of the entire family of curves (the singular integral).

A general integral is the envelope obtained by changing \( A \) while holding \( \phi \) fixed. That is, a linear sweep of the surfaces and is given by

\[ ax + by + c = \sqrt{a^2 + b^2} \int \frac{dz}{\sqrt{(f(z)/F(z))^2 - 1}} \]  

(8.13)
Another general integral is the envelope obtained by changing only $\phi$. This is equivalent to a rotational sweep about the $z$ axis and gives

$$r = \int \frac{dz}{\sqrt{(f'(z)/F(z))^2 - 1}} \quad (8.14)$$

These general integrals can also be obtained directly by looking for solutions of the form $z = G(au + bv + c)$ and $z = G(r)$ respectively.

More complicated non-smooth solutions can be constructed by piecing together parts of these general curves in a continuous manner analogous to that used in Chapter 3.

**Example 19.** The solution to Helmholtz’s equation in three dimensions in the half-space $z > 0$ with $\nabla \eta \cdot \hat{n} = 1$ on $z = 0$ and bounded behaviour as $z \to +\infty$ is $\eta = e^{-z}$. This case has $f = e^{-z}$ and $F = 1$, giving the traced boundaries as

$$\cos \phi x + \sin \phi y + C = \int \frac{dz}{\sqrt{e^{-2z} - 1}} = \arccos e^{-z} \quad (8.15)$$

This can be inverted to give

$$z = \log \cos(\cos \phi x + \sin \phi y + C) \quad (8.16)$$

This is similar to the solution obtained for Helmholtz’s equation in the half-plane where $y = \log \cos(\pm x + C)$. Other solutions can be obtained in three dimensions such as the radially symmetric solutions

$$z = \log \cos(r + C) \quad (8.17)$$

**8.1.2 Spherical Symmetry** If $\eta = \eta(r)$ and $F = F(\eta, \eta_r, r)$ then we can find general solutions for the boundary tracing equations.

This section takes a more constructional approach to generating the general solution.

First a special solution is constructed which remains a solution under rotation about the origin. Thus we have constructed a solution containing two arbitrary constants, i.e. a complete integral. Envelopes of these special solutions are the general integrals and singular integrals which also satisfy the boundary conditions.

A single special solution is found by solving the equation in spherical coordinates $(r, \theta, \phi)$.

$$x = r \cos \theta \quad y = r \sin \theta \cos \phi \quad z = r \sin \theta \sin \phi \quad (8.18)$$
Assuming the surface takes the form \( r(\theta) \) and is symmetric in \( \phi \), the surface normal is given by

\[
\mathbf{n} = \frac{1}{\sqrt{r_\theta^2 + r^2}} \begin{pmatrix}
\sin \theta \\
- \cos \theta \cos \phi \\
- \cos \theta \sin \phi
\end{pmatrix} + r \begin{pmatrix}
\cos \theta \\
\sin \theta \cos \phi \\
\sin \theta \sin \phi
\end{pmatrix}
\]  

(8.19)

We can also calculate \( \nabla \eta \) giving

\[
\nabla \eta = \eta_r \begin{pmatrix}
\cos \theta \\
\sin \theta \cos \phi \\
\sin \theta \sin \phi
\end{pmatrix}
\]  

(8.20)

Putting these into the boundary condition gives an equation for \( r_\theta \).

\[
\nabla \eta \cdot \mathbf{n} = \frac{\eta_r r}{\sqrt{r_\theta^2 + r^2}} = F(r)
\]  

(8.21)

This can be integrated to give

\[
\theta = C \pm \int \frac{|F|}{r \sqrt{\eta_r^2 - F^2}} \, dr
\]  

(8.22)

This surface is symmetric about the \( \phi = 0 \) axis. Since we have spherical symmetry we can rotate the whole surface so that its axis of symmetry points in an arbitrary direction. The freedom to choose this direction is equivalent to the two constants required for a complete integral.

As in Subsection 8.1.1, the general smooth solutions to the spherical symmetry are obtained as envelopes of one parameter sub-families of these special solutions. More general solutions can be created by piecing together sections of these in a continuous manner.

**Example 20.** The radial solution \( \eta = \frac{1}{2}(x^2 + y^2 + z^2) = r^2/2 \) is a solution to Poisson’s equation in three dimensions. For the boundary condition \( \nabla \eta \cdot \mathbf{n} = 1 \) the “special” solution is given by

\[
\theta + C = \int \frac{dr}{r \sqrt{r^2 - 1}} = \arcsin (r^{-1})
\]  

(8.23)

This is equivalent to \( r \sin(\theta + C) = 1 \). As we only need a single solution we can choose \( C = \pi/2 \). In this case the boundary is given by the plane \( x = 1 \). Since a complete integral is obtained by rotating this solution about the origin, a complete integral is given by the planes tangent to the unit sphere. That is for \( A^2 + B^2 + C^2 = 1 \),

\[
Ax + By + Cz = 1
\]  

(8.24)
Thus solution boundaries include (but are not limited to) the unit sphere, Platonic solids, and various other polytopes. An analogous result was mentioned in Subsection 4.2.5.

8.2 Failure for Higher Order PDEs and Systems of PDEs

Boundary tracing fails for PDEs of higher order and systems of PDEs in two dimensions. The problem lies not with the PDE itself but with the associated boundary conditions. Typically for a fourth order PDE, or a system of two linked second order PDEs there are two boundary conditions to be satisfied. This results in two ODEs which must be satisfied by the boundary curve. Thus the system of equation for the boundary is over determined and we obtain no solutions (except in degenerate cases).

8.3 Higher Dimensional Systems of PDEs

In this section we look at the behaviour of systems of PDEs in more than two dimensions. In particular we will focus on the case with two boundary conditions in three dimensions. The extensions to higher dimensions follow in exactly the same manner. The most general case will be looked at in Section 8.3.3.

8.3.1 Two Boundary Conditions in Three Dimensions

Here we look at a dual system using two prescribed functions \( \eta \) and \( \mu \), and two boundary conditions

\[
\nabla \eta \cdot \hat{n} = F \tag{8.25}
\]

\[
\nabla \mu \cdot \hat{n} = G \tag{8.26}
\]

In this case there are two viable cones for the choices of \( \hat{n} \), one for equation (8.25) and one for (8.26). Both conditions must hold for \( \hat{n} \); geometrically \( \hat{n} \) must fall in the intersection of these two cones. Thus, for a valid boundary to exist at some point a variety of conditions must hold.

1. The viable cone for \( \eta \) must exist.
2. The viable cone for \( \mu \) must exist.
3. The two cones must intersect at a point other than 0.

A typical situation is shown in Figure 8.2.

Thus the conditions to be satisfied are

\[
\nabla \eta^2 - F^2 > 0 \quad \nabla \mu^2 - G^2 > 0 \quad |\alpha_1 - \alpha_2| \leq \phi \leq |\alpha_1 + \alpha_2|.
\]

Higher order PDEs can be dealt with by rewriting them as a system of PDEs.
Figure 8.2: The intersection of two dual cones gives two normal directions for the traced surface. The two large arrows represent $\nabla \eta$ and $\nabla \mu$, the smaller arrows the two allowable normals.

The last of these is the requirement that the cones intersect. Here the cone angles are $\alpha_1$ and $\alpha_2$ while $\phi$ is the angle between the cone axes. These are given by:

$$
cos \alpha_1 = \frac{F}{||\nabla \eta||} \quad cos \alpha_2 = \frac{F}{||\nabla \mu||} \quad cos \phi = \frac{\nabla \nu \cdot \nabla \eta}{||\nabla \mu|| \ ||\nabla \eta||}$$

The two geometries where the last condition fails are shown in Figure 8.3.

Each of these conditions is effectively a terminal surface, so we have more than one type of terminal surface.

Considering a point which satisfies these conditions, the intersection of the two viable cones gives us two directions, one on either side of the plane spanned by $\nabla \mu$ and $\nabla \eta$. Consequently we expect two solution surfaces through every point in the viable domain.

While it would be instructive to have simple examples of such surfaces, this is not as easy as it was for boundary tracing in the plane.

8.3.2 The Problem With Symmetry Increasing the dimension from two to three allows additional flexibility, sufficient to solve problems with two simultaneous boundary conditions. Symmetry destroys this flexibility.

The problem is that for solution normals to exist it is necessary that

$$|\alpha_1 - \alpha_2| \leq \phi \leq |\alpha_1 + \alpha_2|$$

If $\mu$ and $\eta$ are symmetric (having the same symmetry) then $\nabla \eta$ and $\nabla \mu$ are
parallel. Thus $\phi = 0$, so (8.28) cannot be satisfied. The geometry of the viable cones can be seen in Figure 8.4.

What does this mean in terms of the (analytic) solvability for higher dimensional higher order problems? It seems that in the cases where we would expect to be able to find analytic solutions, the highly symmetric cases, no traced boundaries exist.

It may be possible to overcome this in the case where $\mu$ and $\eta$ are symmetric but not with the "same" symmetry. Possibly the types of symmetry differ or have different centers/directions.

8.3.3 Interplay Between Dimension and Order The results of Subsection 8.3.1 can be generalised to higher dimensions relatively easily.

Consider boundary tracing in $\Omega \subset \mathbb{R}^M$ with $N$ base functions, $u^1, u^2, \ldots, u^N$, each with its own boundary conditions. These boundary conditions look like.

$$\nabla u^1 \cdot \hat{n} = F_1 \quad (8.29)$$

$$\ldots \quad (8.30)$$

$$\nabla u^N \cdot \hat{n} = F_N \quad (8.31)$$

except in the degenerate case $\alpha_1 = \alpha_2$
8.3. Higher Dimensional Systems of PDEs

Figure 8.4: When $\nabla \eta$ and $\nabla \mu$ are aligned, as in the case where $\eta$ and $\mu$ share symmetry, the viable cone cannot intersect non-degenerately.

Writing $\mathbf{n} = (n_1, n_2, \ldots, n_M)$ and $\nabla u^i = (u_1^i, u_2^i, \ldots, u_M^i)$ we obtain the equations

\[
\begin{align*}
    n_1 u_1^1 + n_2 u_2^1 + \ldots + n_M u_M^1 &= F_1 \\
    n_1 u_1^2 + n_2 u_2^2 + \ldots + n_M u_M^2 &= F_2 \\
    &\vdots \\
    n_1 u_1^N + n_2 u_2^N + \ldots + n_M u_M^N &= F_M \\
    n_1^2 + n_2^2 + \ldots + n_M^2 &= 1
\end{align*}
\]

This is a set of $N + 1$ equations in $M$ variables. Naïvely we might expect isolated solutions at each point when $N + 1 = M$, infinitely many solutions at each point when $N + 1 < M$, and no solutions when $N + 1 > M$. This is consistent with what was found earlier in this chapter.

This simple explanation fails to explain the existence of non-viable domains and terminal curves. Further details can be derived when we look at the structure of the equations more closely. Each of the boundary conditions is essentially a linear equation for $\mathbf{n}$. Thus the normal, if it exists, must be a point in some affine subspace, $\mathbf{L}$, of $\mathbb{R}^M$. Since $\mathbf{n}$ must be a unit vector, it must be in the intersection of $\mathbf{L}$ and the unit sphere.

For different $\mathbf{x} \in \Omega$, $\mathbf{L}$ takes different positions. When $\mathbf{L}$ intersects the unit sphere the point $\mathbf{x}$ is in the viable domain. When $\mathbf{L}$ is tangential to the unit sphere the point $\mathbf{x}$ is on the terminal curve, otherwise $\mathbf{x}$ is outside the viable domain.

A special case occurs when $\mathbf{L}$ is a line, which happens when all the boundary conditions are independent at the point and $N + 1 = M$. In this case the line
Chapter 8. Higher Order and Higher Dimensional Equations

intersects the unit sphere in either zero, one or two points. When \( L \) has dimension greater than one we have either zero, one or an infinite number of normal directions.

Since the behaviour is determined by the affine subspace defined by the boundary conditions, problems can occur at points where the boundary conditions are not linearly independent. At such points the affine subspace either does not exist, or has higher dimension than expected. This means there can be either no solutions or infinitely many solutions for \( \mathbf{n} \). Points where this occurs are kinds of critical points.

The breakdown of boundary tracing for symmetric higher order PDEs in higher dimensions is due the boundary conditions being linearly dependent everywhere in the domain.

8.4 Conclusion

There is a complex interplay between dimension and PDE order for boundary tracing. In this chapter we have introduced two different (but equivalent) ways of considering this interplay: viable cones and the intersection of an affine subspace with a unit \( n \)-sphere.

Increasing the dimension allows more flexibility by increasing the dimension of the viable cone(s). Increasing the PDE order reduces the flexibility by increasing the number of cones.

In higher dimensions there are additional constraints on the viable domain. Some of these constraints are related to the condition in the plane, that viable cones exist. The other constraints correspond to the need for these viable cones to intersect.

Boundary tracing in higher dimensions has been shown to be richer than boundary tracing in the plane and correspondingly more complicated. The possibilities for boundary tracing in such contexts remain open to inquiry.
Discussion and Conclusion

9.1 Discussion

Although boundary tracing is not a new technique, it is not frequently used. This thesis is the first systematic investigation of the technique and also demonstrates the technique's power. As such the thesis was distributed between two areas: development of consistent methods and terminology for boundary tracing, and examples of the results obtainable through boundary tracing.

9.1.1 The Boundary Tracing Framework In Chapter 3 boundary tracing was considered for “general flux” boundary conditions, $\nabla \eta \cdot \hat{n} = F$. It was seen that many features of the boundaries geometry could be determined easily from the base function $\eta$ and $F$. In particular boundary direction and curvature could be expressed easily at any point where $||\nabla \eta|| > |F|$. The curves where $||\nabla \eta|| = |F|$ were called the terminal curves and divided the domain into the viable ($||\nabla \eta|| > |F|$) and nonviable ($||\nabla \eta|| < |F|$) regions. Further expressions for boundary behaviour near terminal curves were developed. These concepts allow an understanding of how traced boundaries behave, as well as providing simple techniques to perform a variety of calculations.

Geometric understanding of the behaviour of traced boundaries near the terminal curves was advanced in Section 3.3 where the traced boundaries were considered as curves on an associated manifold, $z^2 = ||\nabla \eta||^2 - F^2$.

Exact expressions for the traced boundaries were developed for symmetric base functions in Section 3.5. Similar results were obtained in Section 3.6 for asymptotic behaviour near a variety of singularities. These allow direct calculation of traced boundary curves for the commonly occurring case of symmetric base functions. This means that a single simple symmetric solution can lead to a variety of interesting traced domains with exactly known boundaries.

Boundary tracing was extended into higher dimensions and higher order equations in Chapter 8. The application of these techniques to symmetric solutions was investigated in three dimensions. General results concerning the viability of boundary tracing in higher dimensions for higher order PDEs were produced. However this area remains one where further research could be conducted.

9.1.2 The Utility Of Boundary Tracing The utility of boundary tracing can be seen through the wide variety of interesting results obtained in the examples in Chapter 4, the consideration of Helmholtz’s equation and the Laplace–Young
equation in Chapters 5 and 6 respectively and the results for rounded corners in Chapter 7. These results are derived using new and interesting domains obtained by boundary tracing.

The wide variety of boundary behaviour obtainable through boundary tracing were shown in examples in Chapter 4.

In particular it was shown that boundary tracing can produce domains with corners and these can lead to new information about the PDE. This technique is of wide applicability and requires the knowledge of only relatively simple solutions.

In Chapter 5 and Chapter 6 boundary tracing was used to derive behaviour of rough surfaces for Helmholtz’s equation and the Laplace–Young equation. It was seen in both these cases that the effect of a microscopically rough boundary was a change in a single parameter of the large scale boundary condition.

9.2 Conclusion

The aim of this thesis has been twofold: to illustrate the power of boundary tracing for real-world problems and to develop a consistent terminology and methodology for its use.

The general techniques developed in Chapter 3 include expressions concerning boundary existence and geometry, and facilitate an intuitive understanding of traced boundary behaviour. These results are used on a wide spectrum of examples in Chapters 4 to 7. These examples range from simple base functions without associated PDE to solutions of the nonlinear Laplace–Young equation. While these examples provide many new results, the results for domains with rounded corners or rough-edges and the new results for the nonlinear Laplace–Young problem were notable. Boundary tracing is likely to be of most use in similar situations, where standard techniques fail, such as when the problem is nonlinear or in situations with complicated geometry.

Although only two dimensional, second order elliptic PDEs are considered in depth, boundary tracing is not restricted to these cases. Extensions to higher dimensions and higher order PDEs are considered in Chapter 8. These preliminary investigations suggest that while boundary tracing becomes more complicated for higher order, higher dimension problems, it remains a feasible technique.

While boundary tracing has been used previously in an ad hoc manner, this thesis has shown that it is a simple and generally applicable tool that can be used on many difficult real-world problems.
Generating The Images

This chapter details some of the variety of techniques used to generate the images in this thesis. This will be split into two sections, the numerical methods for generating the boundaries and the techniques used to visualise them.

Most of the calculations were performed on a PII-450 running linux. The visualisations were done on the same machine using MS Windows software.

A.1 Numerical Boundary Tracing

There were two types of boundary tracing used in generating the images. The first of these was restricted to the plane. The second was on the associated manifold.

A.1.1 Tracing In The Plane Since we are working in two dimensions, two equations for the boundary are needed. These come from the boundary condition \( \nabla \eta \cdot \hat{n} = F \) and a parametrisation choice. Arc-length parameterisation was found to work well, so the boundary tracing equations are

\[
-\eta_y \dot{x} + \eta_x \dot{y} = \pm F \\
\dot{x}^2 + \dot{y}^2 = 1
\]  

(A.1)  

(A.2)

One problem with this is that at any given \((x,y)\) there are four, two or zero choices for \((\dot{x}, \dot{y})\), depending on whether \((x,y)\) is inside the viable domain, on the terminal curve or outside the viable domain.

Integration was done using a 5th-6th order Runge-Kutta method with adaptive step size. The choice for \((\dot{x}, \dot{y})\) was the one closest to the previous value, thus ensuring smoothness of the curve.

The integrations were carried out using Mathematica, Matlab or, when speed was important, custom written C++ code.

Problems occurred when the traced curves hit the terminal curves. These problems were partly due to Mathematica and Matlab continuing to solve ODEs using complex numbers outside the viable domain. This was fixed by terminating the calculation when the curve went outside the viable domain.

A.1.2 Tracing On The Manifold Here the ODE required is three dimensional, thus we need an extra condition, and this condition is related to keeping the curve on the manifold.

Letting \( G = \|\nabla \| - F^2 - z^2 \), then the manifold is given by \( G = 0 \). This suggests that an appropriate choice for the extra condition would be \( \dot{G} = -\lambda G \) for \( \lambda > 0 \).
Thus the system of equations becomes

\[ \nabla \eta \cdot \hat{n} = F \] (A.3)
\[ x^2 + y^2 + z^2 = 1 \] (A.4)
\[ \dot{G} = -\lambda G \] (A.5)

In this case there is again 4 directions at most points. This can be reduced to two on each “half” of the manifold, by projecting the branches of the direction field onto the manifold. One consistent method of doing this is by rotation; choosing the direction to the left of \( \nabla \eta \) on the top half and that to the right on the lower half. The decision between the forward direction and the backward direction was made by comparison with the previous direction.

The integration was done with a simple custom written Runge–Kutta method implemented in octave, a free GNU clone of Matlab.

Generation of curves for the images typically required one half to two hours per image (depending on the base function, desired detail, number of curves etc.)

A.2 Visualising The Data

The output of the ODE integrators consisted of large numbers of points. These points were then imported into the NURBS modeling package Rhino where the curves were converted from lists of thousands of points, into NURBS curves with far fewer points.

The resulting curves were exported, in the IGES modeling format, to be read by the modeler 3D Studio MAX for rendering.

Conversion of point lists to NURBS typically required approximately 10 minutes per image, and rendering 30 to 45 minutes per image.
Elliptic Integrals

Three elliptic integrals and the Jacobi Elliptic functions are introduced here. These functions are required to express the solutions to various ODEs that arise in this thesis. There are many notations used for these functions. We shall use the definitions presented in Mathematica.

\[ F(\phi | m) = \int_{0}^{\phi} (1 - m \sin^2 \theta)^{-1/2} d\theta \]  
\[ \Pi(n; \phi | m) = \int_{0}^{\phi} (1 - n \sin^2 \theta)^{-1}(1 - m \sin^2 \theta)^{-1/2} d\theta \]  
\[ E(\phi | m) = \int_{0}^{\phi} (1 - m \sin^2 \theta)^{1/2} d\theta \]

The reason for using these functions is that they allow a simple representation of several types of integrals which occur in this work

\[ \int \frac{dx}{\sqrt{x^2 - A^2 \sqrt{x^2 - B^2}}} = \frac{1}{B} F \left( \text{arcsin} \left( \frac{x}{A} \right) | \frac{A^2}{B^2} \right) \]
\[ \int \frac{dx}{\sqrt{x^2 - A^2 \sqrt{x^2 - B^2}(x^2 - C^2)}} = \frac{1}{AC^2} \Pi \left( \frac{B^2}{C^2}; \text{arcsin} \left( \frac{x}{B} \right) | \frac{B^2}{A^2} \right) \]
\[ \int \frac{\sqrt{x^2 - A^2}}{\sqrt{x^2 - B^2}} \, dx = AE \left( \text{arcsin} \left( \frac{x}{B} \right) | \frac{B^2}{A^2} \right) \]

The elliptic F function is the inverse of the Jacobi Amplitude function. That is if \( \varphi = \text{am}(u | m) \) then \( u = F(\varphi | m) \)

The Jacobi Elliptic functions \( \text{sn}(u | m) \) and \( \text{cn}(u | m) \) are given by

\[ \text{sn}(u | m) = \sin(\text{am}(u | m)) \]
\[ \text{cn}(u | m) = \cos(\text{am}(u | m)) \]
\[ \text{dn}(u | m) = \sqrt{1 - m^2 \text{sn}^2(u | m)} \]

Additional Jacobi elliptic functions are defined in terms of these. (Although only a few of these are needed, the complete list is included)

\[ \text{ns}(u | m) = 1/\text{sn}(u | m) \]
\[ \text{nc}(u | m) = 1/\text{cn}(u | m) \]
\[ \text{nd}(u | m) = 1/\text{dn}(u | m) \]
\[ \text{sc}(u | m) = \text{sn}(u | m)/\text{cn}(u | m) \]
\[ \text{sd}(u | m) = \text{sn}(u | m)/\text{dn}(u | m) \]
\begin{align*}
cs(u \mid m) &= \frac{\cn(u \mid m)}{\sn(u \mid m)} \\
cd(u \mid m) &= \frac{\cn(u \mid m)}{\dn(u \mid m)} \\
ds(u \mid m) &= \frac{\dn(u \mid m)}{\sn(u \mid m)} \\
dc(u \mid m) &= \frac{\dn(u \mid m)}{\cn(u \mid m)}
\end{align*}
Figure C.1: The surface $z^2 = \nabla \eta^2 - F^2$ (denoted M) takes two $z$ values, for each point in the viable domain (V) but none in the non-viable domain (NV). It intersects the $z = 0$ plane at the terminal curve (T).
Figure C.2: A traced boundary (A) in the plane with a cusp at the point P on the terminal curve can be considered a smooth curve (B) on the surface $z^2 = \nabla \eta^2 - F^2 (M)$.

Figure C.3: The traced boundaries, shown in two dimensions and on the associated manifold, for $\eta = \sin \rho x \sin \mu y$ with the boundary condition $\nabla \eta \cdot \mathbf{n} = c$ with $c_1 < c < c_{MAX}$, form balls.
Figure C.4: The traced boundaries, shown in two dimensions and on the associated manifold, for $\eta = \sin \rho x \sin \mu y$ with the boundary condition $\nabla \eta \cdot \hat{n} = c$ and $0 < c < c_1$, form a connected “mesh”.

Figure C.5: The solution inside an equilateral triangle for the Poisson’s equation. Left: Top view showing the terminal circle $r = \frac{2c}{K}$ and the triangular domain. Right: Three dimensional figure showing the solution, viable (blue) and nonviable domains (red). (See Figure C.5 for colour version)
Figure C.6: Image of the three dimensional solution for Helmholtz's equation in a domain with a sharp corner, constructed by boundary tracing.

Figure C.7: Image of the three dimensional solution for Helmholtz's equation in a domain with a re-entrant sharp corner, constructed by boundary tracing.
Figure C.8: **Image** showing a “rough” surface and solution produced by boundary tracing. Grey lines in the left figure are full traced boundary curves.

Figure C.9: **A corner** formed from traced curves with different boundary conditions.

Figure C.10: **Numerical results** to Helmholtz’s equation in a traced domain. **Left:** The solution calculated using finite elements. **Right:** The difference between the exact solution $e^{-y}$ and the numerical solution.
Figure C.11: **Left:** An annular solution to Helmholtz's equation, with its traced counterpart. Note the height rise into the corners. **Right:** The two solutions match together smoothly.

Figure C.12: **Typical domains obtained from numerically boundary tracing the solution to the Laplace–Young equation in an annulus. Left:** A three dimensional view of the domain with cut-away showing solution behaviour. **Right:** Top view of a simple domain.
Bibliography


