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Trefftz Methods for Time Dependent Partial Differential Equations

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Abstract: In this paper we present a mesh-free approach to numerically solving a class of second order time dependent partial differential equations which include equations of parabolic, hyperbolic and parabolic-hyperbolic types. For numerical purposes, a variety of transformations is used to convert these equations to standard reaction-diffusion and wave equation forms. To solve initial boundary value problems for these equations, the time dependence is removed by either the Laplace or the Laguerre transform or time differencing, which converts the problem into one of solving a sequence of boundary value problems for inhomogeneous modified Helmholtz equations. These boundary value problems are then solved by a combination of the method of particular solutions and Trefftz methods. To do this, a variety of techniques is proposed for numerically computing a particular solution for the inhomogeneous modified Helmholtz equation. Here, we focus on the Dual Reciprocity Method where the source term is approximated by radial basis functions, polynomial or trigonometric functions. Analytic particular solutions are presented for each of these approximations. The Trefftz method is then used to solve the resulting homogenous equation obtained after the approximate particular solution is subtracted off. Two types of Trefftz bases are considered, F-Trefftz bases based on the fundamental solution of the modified Helmholtz equation, and T-Trefftz bases based on separation of variables solutions. Various techniques for satisfying the boundary conditions are considered, and a discussion is given of techniques for mitigating the ill-conditioning of the resulting linear systems. Finally, some numerical results are presented illustrating the accuracy and efficacy of this methodology.

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1 Introduction

Traditional methods for numerically solving partial differential equations (PDEs) such as the finite difference, finite element and boundary element methods all require meshing some or all of the solution domain [Strang and Fix (1973); Partridge, Brebbia and Wrobel (1992); Golberg and Chen (1996)]. This can be extremely time consuming, particularly for problems in $\mathbb{R}^3$and can severely limit the attainable accuracy because meshing the domain boundary can usually be done with only limited accuracy [Strang and Fix (1973); Partridge, Brebbia and Wrobel (1992); Golberg and Chen (1996)]. Consequently, over the past decade there has been increasing interest in developing meshless methods which eliminate or substantially reduce the need for domain meshing. Among these methods are the element-free Galerkin method [Belytschko and Lu (1994)], reproducing kernel particle methods [Liu, Jun, Li, Adee and Belytschko (1995)], the local Petrov-Galerkin method and methods based on radial basis function approximations [Kansa (1990a, 1990b)]. With the exception of the latter, all the other methods require at least some meshing for numerical integration, hence are more realistically mesh reduced, rather than mesh-free methods. Interestingly, for many years during the 50's, 60's and 70's a popular class of methods was the Trefftz methods introduced in 1926 [Trefftz (1926)] which are based on approximating solutions by generalized Fourier series. These methods are truly meshless, since they can be implemented without either domain or surface meshing. Unfortunately, their use was limited largely to the solution of homogeneous elliptic equations such as the Laplace, Helmholtz and biharmonic equations. However, in recent years, extensive research on the numerical evaluation of particular solutions to PDEs based on early research of [Nardini and Brebbia (1982)] and [Atkinson (1985)] has enabled one to extend these methods to solve inhomogeneous elliptic [Fairweather and Karageorghis (1998); Golberg and Chen (1998)], nonlinear [Golberg and Chen (1998)] and

time dependent PDEs [Golberg and Chen (1998)]. It is the purpose of this paper to present a meshless approach to solving a class of second order time-dependent PDEs based on a combination of the method of particular solutions and the Trefftz method.

The paper is composed of eight sections. In Section 2 we present boundary value problems (BVPs) for a class of second order PDEs which contains parabolic, hyperbolic and parabolic-hyperbolic equations. By using a variety transformations we show how to reduce these equations to familiar reaction-diffusion and wave equation forms. In addition to standard Dirichlet, Neumann and mixed boundary conditions, we consider a class of recently discussed nonlocal boundary conditions and the solution of boundary value problems for functionally graded materials [Paulino, Sutradhar and Gray (2002); Sutradhar, Paulino and Gray (2002)].

In Section 3 we show how to reduce the solution of the standard time dependent PDEs to solving BVPs for the inhomogeneous modified Helmholtz equation. We discuss three methods for doing this; the Laplace transform [Moridis (1987)], various time-differencing schemes [Su and Tabarrok (1997); Ingber and Phan-Thien (1992); Chapko and Kress (1997)] and the Laguerre transform [Chapko and Kress (2000)].

In Section 4 we introduce the method of particular solutions (MPS) to reduce the inhomogeneous modified Helmholtz equation to BVPs for the homogeneous modified Helmholtz equation. Here we assume that the necessary particular solutions are known and focus on the general Trefftz method for solving homogeneous BVPs. In particular, we concentrate on methods for satisfying the boundary conditions. A variety of methods is discussed; collocation, least squares and Galerkin's method, with Galerkin's method appearing to be the most reliable.

In Section 5 we turn to the issue of numerically evaluating particular solutions to the inhomogeneous modified Helmholtz equation. Two general approaches are discussed. The direct numerical calculation of the classical domain integral [Partridge, Brebbia and Wrobel (1992); Golberg and Chen (1996)] and the currently more popular Dual Reciprocity Method (DRM) [Partridge, Brebbia and Wrobel (1992); Golberg and Chen (1996)]. Here, the source term is approximated by an appropriate set of basis functions and then an approximate particular solution is obtained by analytically solving the modified Helmholtz equation with the approximate source term. Three types of approximations are considered: *radial basis functions* (RBFs), polynomials [Golberg, Muleshkov, Chen and Cheng (2003); Muleshkov, Chen, Golberg and Cheng (2000)] and trigonometric approximations [Li and Chen (2004)]. Advantages and disadvantages are discussed.

In Section 6 we return to a discussion of specific Trefftz bases. Two general classes of bases are considered, F-Trefftz bases based on fundamental solutions of the modified Helmholtz equation [Golberg, Muleshkov, Chen and Cheng (2003)] and T-Trefftz bases which are generally obtained by separation of variables in polar and Cartesian coordinate systems [Cheung, Jin and Zienkiewicz (1991); Discroll (1995); Melenk (1995); Melenk and Babuška (1995)]. For two dimensional problems we show how Bergman-Vekua operators can be used to obtain error estimates for T-Trefftz bases [Bergman and Herriot (1965); Vekua (1967); Melenk (1995); Melenk and Babuška (1995)].

In Section 7 we present some numerical examples to show the efficacy and efficiency of our approach. We conclude the paper with some discussion of future research in this area.

2 Boundary Value Problems for Time Dependent PDEs

In this paper we consider the numerical solution of initial boundary value problems for a class of second order partial differential equations (PDEs) of the form

$$\sum_{j=1}^{2}\sum_{i=1}^{2} a_{ij}\frac{\partial^2 u}{\partial x_i \partial x_j}+\sum_{i=1}^{2} k_i\frac{\partial u}{\partial x_i}-cu=a\frac{\partial u}{\partial t}+b\frac{\partial^2 u}{\partial t^2}+f \text{ in } \mathbb{R}^2 \tag{2.1}$$

and

$$\sum_{j=1}^{3}\sum_{i=1}^{3} a_{ij}\frac{\partial^2 u}{\partial x_i \partial x_j}+\sum_{i=1}^{3} k_i\frac{\partial u}{\partial x_i}-cu=a\frac{\partial u}{\partial t}+b\frac{\partial^2 u}{\partial t^2}+f \text{ in } \mathbb{R}^3 \tag{2.2}$$

where

$$\mathbf{A}_1=[a_{ij}],\ 1\le i,j\le 2 \tag{2.3}$$

and

$$\mathbf{A}_2=[a_{ij}],\ 1\le i,j\le 3 \tag{2.4}$$

are constant, symmetric, positive definite matrices and (a,b,c) are non-negative constants.

If $b=0$, $a>0$ then (2.1)-(2.2) are *parabolic equations* and if $b>0$, $a\geq 0$ then (2.1)-(2.2) are called *hyperbolic equations*. For numerical purposes, it is convenient to transform (2.1)-(2.2) into a standard form. For parabolic equations, the standard form is the *reaction-diffusion equation*,

$$\frac{\partial^2 u}{\partial x_1^2}+\frac{\partial^2 u}{\partial x_2^2}-cu=\frac{\partial u}{\partial t}+f \text{ in } \mathbb{R}^2 \tag{2.5}$$

and

$$\frac{\partial^2 u}{\partial x_1^2}+\frac{\partial^2 u}{\partial x_2^2}+\frac{\partial^2 u}{\partial x_3^2}-cu=\frac{\partial u}{\partial t}+f \text{ in } \mathbb{R}^3. \tag{2.6}$$

As usual, we will denote the left hand sides of (2.5)-(2.6) as $\Delta u-cu$ where Δ is the Laplacian operator.

For hyperbolic equations the standard form is,

$$\Delta u-cu=\frac{\partial^2 u}{\partial t^2}+f \text{ in } \mathbb{R}^d,\ d=2,3 \tag{2.7}$$

the classical *wave equation*. We consider these cases separately.

2.1 Parabolic Equations

Although one can consider boundary value problems for both bounded and unbounded domains, in this paper we will focus primarily on problems in bounded domains.

Hence, let D be a bounded domain in $\mathbb{R}^d$, $d=2,3$ with boundary S. Denoting the left hand side of (2.1)-(2.2) by Lu, the parabolic equation takes the form

$$Lu=a\frac{\partial u}{\partial t}+f. \tag{2.8}$$

In the initial boundary value problem (IBVP) one specifies, the initial condition

$$u(P,0)=m(P),\ P\in D\cup S \tag{2.9}$$

and boundary conditions

$$Bu(P,t)=g(P,t),\ P\in S \tag{2.10}$$

where B is an appropriate boundary operator. The most common forms of boundary conditions are, Dirichlet boundary conditions,

$$Bu=u; \tag{2.11}$$

Neumann boundary conditions where

$$Bu=\frac{\partial u}{\partial \mathbf{n}_c} \tag{2.12}$$

and $\partial u/\partial \mathbf{n}_c$ is the *conormal derivative* of u. Here,

$$\frac{\partial u}{\partial \mathbf{n}_c}=\text{grad}u\cdot \mathbf{n}_c \tag{2.13}$$

where $\mathbf{n}_c$ is the conormal at $P\in S$. Specifically, if $\mathbf{A}$ is as in (2.3)-(2.4) then

$$\mathbf{n}_c=\mathbf{An}=\left(\sum_{j=1}^{d}a_{ij}n_j\right),\ 1\leq i\leq d \tag{2.14}$$

where $\mathbf{n}=(n_i)$, $1\leq i\leq d$ is the unit outward normal at $P\in S$.

Mixed Boundary Conditions:

Here, we assume that $S=S_1\cup S_2$, $S_1\cap S_2=\emptyset$ and one specifies Dirichlet boundary conditions on S_1 and Neumann boundary conditions on S_2. If g_1 and g_2 are the corresponding boundary conditions, and $w(P)=1$, $P\in S_1$ and $w(P)=0$, $P\in S_2$, then these boundary conditions can be written in the form

$$wu+(1-w)\frac{\partial u}{\partial \mathbf{n}_c}=wg_1+(1-w)g_2. \tag{2.15}$$

In fact, if $P\in S_1$, then $w=1$, $1-w=0$ so (2.15) becomes

$$u=g_1, \tag{2.16}$$

while if $P\in S_2$, $w=0$, $1-w=1$ and (2.15) becomes

$$\frac{\partial u}{\partial \mathbf{n}_c}=g_2. \tag{2.17}$$

Hence, letting $g=wg_1+(1-w)g_2$ (2.15) can be written as

$$Bu=g \tag{2.18}$$

where $Bu=wu+(1-w)\partial u/\partial \mathbf{n}_c$.

One can also consider boundary conditions of the third kind - Robin boundary conditions

$$\frac{\partial u}{\partial \mathbf{n}_c}=\alpha(P)u+g \tag{2.19}$$

where

$$Bu=\frac{\partial u}{\partial \mathbf{n}_c}-\alpha(P)u. \tag{2.20}$$

One can also consider non-linear boundary conditions, such as radiation boundary conditions

$$\frac{\partial u}{\partial \mathbf{n}_c} = \alpha u^4. \tag{2.21}$$

However, in this paper we will only deal with the case where B is linear.

Under appropriate smoothness conditions on S, f and g and compatibility conditions on the initial and boundary data, one can show that (2.8)-(2.10) have unique solutions. For details one can consult [Friedman (1964)]. We will assume that these conditions are met in the remainder of the paper.

Although (2.8)-(2.10) represent classical IBVPs, in recent years a number of authors have considered non-local conservation conditions on u of the form [Cannon and Lin (1990); Ang (2002)]

$$\int_D u(P,t)\,dV = h(t). \tag{2.22}$$

When (2.8) is in the standard form (2.5)-(2.6) with $c = f = 0$, this condition can be converted to a non-local boundary condition on S as follows.

Assuming h in (2.22) is differentiable, we differentiate (2.22) giving

$$\int_D \frac{\partial}{\partial t} u(P,t)\,dV = h'(t). \tag{2.23}$$

From (2.5)-(2.6) $\partial u/\partial t = \Delta u$ so that

$$\int_D \Delta u(P,t)\,dV = h'(t) = \int_D div\text{grad}u(P,t)\,dV. \tag{2.24}$$

Now, by using the divergence theorem,

$$\begin{aligned}&\int_D div\text{grad}u(P,t)\,dV\\ &= \int_S \mathbf{n}\cdot \text{grad}u(P,t)\,dS = \int_S \frac{\partial u}{\partial \mathbf{n}}(P,t)\,dS.\end{aligned} \tag{2.25}$$

Hence, the conservation condition (2.22) is equivalent to the non-local boundary condition

$$\int_S \frac{\partial u}{\partial \mathbf{n}}(P,t)\,dS = h'(t). \tag{2.26}$$

Some existence and uniqueness theorems for this class of BVPs are given in [Cannon and Lin (1990)] and numerical methods can be found in [Ang (2000, 2002)].

2.1.1 Conversion to Standard Form

To convert (2.1)-(2.2) to standard form we begin by eliminating the mixed derivatives in (2.1)-(2.2). To do this, we first observe that we can write

$$\sum_{j=1}^{d}\sum_{i=1}^{d} a_{ij}\frac{\partial^2 u}{\partial x_i \partial x_j} = div(\mathbf{A}\text{grad}u) \tag{2.27}$$

where $\mathbf{A}$ is given in (2.3)-(2.4). Since $\mathbf{A}$ is symmetric, it follows that

$$\mathbf{A} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^T \tag{2.28}$$

where $\mathbf{U}$ is orthogonal and $\mathbf{\Lambda}$ is a diagonal matrix of eigenvalues of $\mathbf{A}$. Thus,

$$\begin{aligned}&div(\mathbf{A}\text{grad}u) = div\left(\mathbf{U}\mathbf{\Lambda}\mathbf{U}^T\text{grad}u\right)\\ &= \left\langle \text{grad}, \mathbf{U}\mathbf{\Lambda}\mathbf{U}^T\text{grad}u\right\rangle\end{aligned} \tag{2.29}$$

where $\text{grad} \equiv (\partial/\partial x_1, \partial/\partial x_1, \ldots, \partial/\partial x_d)$ and $\langle\cdot,\cdot\rangle$ denotes the inner product of grad with the vector $\mathbf{A}\text{grad}u$. Hence,

$$div(\mathbf{A}\text{grad}u) = \left\langle \mathbf{U}^T\text{grad}, \mathbf{\Lambda}\mathbf{U}^T\text{grad}u\right\rangle. \tag{2.30}$$

Now let

$$\xi = \mathbf{U}\mathbf{x} \tag{2.31}$$

so that

$$\text{grad}_{\mathbf{x}} = \mathbf{U}\text{grad}_{\xi} \tag{2.32}$$

where the subscripts in (2.32) denote the variables of the corresponding gradients. Hence,

$$\langle \text{grad}_{\mathbf{x}}, \mathbf{A}\text{grad}_{\mathbf{x}}u\rangle = \left\langle \text{grad}_{\boldsymbol{\xi}}, \mathbf{\Lambda}\text{grad}_{\boldsymbol{\xi}}u\right\rangle \tag{2.33}$$

Thus,

$$\sum_{j=1}^{d}\sum_{i=1}^{d} a_{ij}\frac{\partial^2 u}{\partial x_i \partial x_j} = \sum_{i=1}^{d}\lambda_i \frac{\partial^2 u}{\partial \xi_i^2} \tag{2.34}$$

where $\lambda_i > 0,\ i = 1,2,\ldots,d$. A further scale change as in (2.42) converts $\sum_{i=1}^{d}\lambda_i \partial^2 u/\partial \xi_i^2$ to diagonal form

$$\sum_{i=1}^{d}\frac{\partial^2 u}{\partial \eta_i^2}. \tag{2.35}$$

Similarly, the first derivative terms get mapped into the form $\sum_{i=1}^{d} k_i' \partial u/\partial \eta_i$ for appropriate values of k_i', $1 \le i \le d$. Thus, these transformations convert Lu to the form

$$Lu = \sum_{i=1}^{d}\frac{\partial^2 u}{\partial \eta_i^2} + \sum_{i=1}^{d} k_i'\frac{\partial u}{\partial \eta_i} - cu \tag{2.36}$$

so that solving (2.1)-(2.2) are equivalent to solving the equation

$$\sum_{i=1}^{d}\frac{\partial^2 u}{\partial x_i^2}+\sum_{i=1}^{d}k_i'\frac{\partial u}{\partial x_i}-cu=a\frac{\partial u}{\partial t}+f. \tag{2.37}$$

In addition to transforming the differential equation to the simpler form (2.5)-(2.6), we need to consider transforming the boundary conditions as well.

First, one observes that the boundary operator for Dirichlet boundary conditions remains unchanged. For Neumann boundary conditions we need to examine how the conormal changes when $\mathbf{x}\to\mathbf{U}^T\boldsymbol{\xi}$. As above, $\mathrm{grad}_{\mathbf{x}}u\to \mathbf{U}\mathrm{grad}_{\boldsymbol{\xi}}u$. Assuming that locally in the neighborhood of P that S is given by the equation $l(P)=0$, for a suitably differentiable function l, then the unit normal at P is given by

$$\mathbf{n}=\frac{\mathrm{grad}_{\mathbf{x}}l}{\|\mathrm{grad}_{\mathbf{x}}l\|} \tag{2.38}$$

where $\|\cdot\|$ is the Euclidean norm of a vector in $\mathbb{R}^d, d=2,3$. Then in the ξ variables

$$\mathbf{n}=\frac{\mathbf{U}\mathrm{grad}_{\boldsymbol{\xi}}l}{\left\|\mathrm{grad}_{\boldsymbol{\xi}}l\right\|} \tag{2.39}$$

and

$$\mathbf{n}_c=\mathbf{A}\left(\frac{\mathbf{U}\mathrm{grad}_{\boldsymbol{\xi}}l}{\left\|\mathrm{grad}_{\boldsymbol{\xi}}l\right\|}\right). \tag{2.40}$$

Thus,

$$\begin{aligned}\frac{\partial u}{\partial \mathbf{n}_c}&=\langle\mathbf{n}_c,\mathrm{grad}_{\mathbf{x}}u\rangle=\frac{\left\langle\mathbf{AU}\mathrm{grad}_{\boldsymbol{\xi}}l,\mathbf{U}\mathrm{grad}_{\boldsymbol{\xi}}u\right\rangle}{\left\|\mathrm{grad}_{\boldsymbol{\xi}}l\right\|}\\&=\frac{\left\langle\mathbf{U}^T\mathbf{AU}\mathrm{grad}_{\boldsymbol{\xi}}l,\mathrm{grad}_{\boldsymbol{\xi}}u\right\rangle}{\left\|\mathrm{grad}_{\boldsymbol{\xi}}l\right\|}=\frac{\left\langle\boldsymbol{\Lambda}\mathrm{grad}_{\boldsymbol{\xi}}l,\mathrm{grad}_{\boldsymbol{\xi}}u\right\rangle}{\left\|\mathrm{grad}_{\boldsymbol{\xi}}l\right\|}\end{aligned} \tag{2.41}$$

Now make the scale transformation

$$\eta_i=z_i/\sqrt{\lambda_i},\ 1\le i\le d, \tag{2.42}$$

so that

$$\left\langle\boldsymbol{\Lambda}\mathrm{grad}_{\boldsymbol{\xi}}l,\mathrm{grad}_{\boldsymbol{\xi}}u\right\rangle=\left\langle\mathrm{grad}_{\boldsymbol{\eta}}l,\mathrm{grad}_{\boldsymbol{\eta}}u\right\rangle$$

and

$$\left\|\mathrm{grad}_{\boldsymbol{\xi}}l\right\|=\left[\frac{1}{\lambda_1}\left(\frac{\partial l}{\partial\eta_1}\right)^2+\frac{1}{\lambda_2}\left(\frac{\partial l}{\partial\eta_2}\right)^2\right]^{1/2},\ \text{in }\mathbb{R}^2 \tag{2.43}$$

and

$$\begin{aligned}&\left\|\mathrm{grad}_{\boldsymbol{\xi}}l\right\|\\&=\left[\frac{1}{\lambda_1}\left(\frac{\partial l}{\partial\eta_1}\right)^2+\frac{1}{\lambda_2}\left(\frac{\partial l}{\partial\eta_2}\right)^2+\frac{1}{\lambda_3}\left(\frac{\partial l}{\partial\eta_3}\right)^2\right]^{1/2},\\&\quad\text{in }\mathbb{R}^3.\end{aligned} \tag{2.44}$$

Let $\alpha(P)$ denote the right-hand sides of (2.43)-(2.44) so that

$$\begin{aligned}\frac{\partial a}{\partial \mathbf{n}_c}&=\frac{\left\langle\mathrm{grad}_{\boldsymbol{\eta}}l,\mathrm{grad}_{\boldsymbol{\eta}}u\right\rangle}{\alpha(P)}=\frac{\left\langle\mathrm{grad}_{\boldsymbol{\eta}}l,\mathrm{grad}_{\boldsymbol{\eta}}u\right\rangle}{\alpha(P)}\cdot\frac{\left\|\mathrm{grad}_{\boldsymbol{\eta}}l\right\|}{\left\|\mathrm{grad}_{\boldsymbol{\eta}}l\right\|}\\&=\frac{\left\langle\mathrm{grad}_{\boldsymbol{\eta}}l,\mathrm{grad}_{\boldsymbol{\eta}}u\right\rangle}{\left\|\mathrm{grad}_{\boldsymbol{\eta}}l\right\|}\cdot\beta(P)\end{aligned} \tag{2.45}$$

where $\beta(P)=\left\|\mathrm{grad}_{\boldsymbol{\eta}}l\right\|/\alpha(P)$. Hence in the η variables,

$$\frac{\partial u}{\partial \mathbf{n}_c}=\beta(P)\frac{\partial u}{\partial \mathbf{n}}. \tag{2.46}$$

Assuming $\mathrm{grad}_{\boldsymbol{\eta}}l\neq 0$ the conormal boundary condition $\partial u/\partial\mathbf{n}_c=g(P)$ is equivalent to the Neumann boundary condition

$$\frac{\partial u}{\partial \mathbf{n}}=g' \tag{2.47}$$

where $g'=g/\beta$.

The remaining step in reducing (2.36)-(2.37) to standard form is to eliminate the first order connective terms in (2.36)-(2.37). For this we define a new dependent variable v by

$$v=\exp\left(-\left\langle\mathbf{k}',\mathbf{x}\right\rangle/2\right)u \tag{2.48}$$

where $\langle\mathbf{k}',\mathbf{x}\rangle=\sum_{i=1}^{d}k_i'x_i$. It can be verified by direct differentiation that v satisfies

$$\sum_{i=1}^{d}\frac{\partial^2 v}{\partial x_i^2}-c'v=a\frac{\partial v}{\partial t}+f' \tag{2.49}$$

for suitable values of $c'>0$ and f'.

Finally, making the scale transformation $\tau = t/a$, $v\langle P,\tau\rangle$ satisfies

$$\sum_{i=1}^{d} \frac{\partial^2 v}{\partial x_i^2} - c'v = \frac{\partial v}{\partial \tau} + f' \tag{2.50}$$

which is the standard form of (2.36)-(2.37).

2.1.2 Functionally Graded Materials

One drawback of Trefftz methods, as for boundary integral methods, is the difficulty of dealing with equations with nonconstant coefficients. However, if it is possible to transform the problem to one with constant coefficients then a Trefftz method may be suitable. An interesting example of this occurs in some recent work on heat transfer in functionally graded materials [Paulino, Sutradhar and Gray (2002); Sutradhar, Paulino and Gray (2002)]. This leads in $\mathbb{R}^3$ to solving the equation

$$div\left(e^{\beta z}\text{grad}u\right) = ke^{\beta z}\frac{\partial u}{\partial t} + f. \tag{2.51}$$

As we show, this equation can be transformed to the standard form of the parabolic differential equation.

From (2.51)

$$\begin{aligned} &div\left(e^{\beta z}\text{grad}u\right) \\ &= \frac{\partial}{\partial x}\left(e^{\beta z}\frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y}\left(e^{\beta z}\frac{\partial u}{\partial y}\right) + \frac{\partial}{\partial z}\left(e^{\beta z}\frac{\partial u}{\partial z}\right) \\ &= e^{\beta z}\frac{\partial^2 u}{\partial x^2} + e^{\beta z}\frac{\partial^2 u}{\partial y^2} + e^{\beta z}\frac{\partial^2 u}{\partial z^2} + \beta e^{\beta z}\frac{\partial u}{\partial z} \end{aligned} \tag{2.52}$$

so (2.51) becomes

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} + \beta\frac{\partial u}{\partial z} = k\frac{\partial u}{\partial t} + e^{-\beta z}f. \tag{2.53}$$

Now (2.53) is of the form of the convection-diffusion equation with $k_1 = k_2 = 0$ and $k_3 = \beta$ so that the transformation $v = e^{-\beta z/2}u$ transforms (2.53) to the standard form (up to a scale transformation) for v.

We note that this equation can be solved using the BEM [Paulino, Sutradhar and Gray (2002); Sutradhar, Paulino and Gray (2002)] - however, as we shall see, our approach allows solution by meshless Trefftz methods.

2.2 Hyperbolic Equations

Using the same coordinate and variable transformations as in the parabolic case, the general hyperbolic equation can be converted to the form

$$\Delta w - cu = a\frac{\partial u}{\partial t} + b\frac{\partial^2 u}{\partial t^2} + f. \tag{2.54}$$

To convert (2.54) to standard form it suffices to eliminate the first order time derivative in (2.54). To do this we define

$$u = e^{\alpha t}v \tag{2.55}$$

and determine α to eliminate the first order time derivative.

Thus,

$$\frac{\partial u}{\partial t} = \alpha e^{\alpha t}v + e^{\alpha t}\frac{\partial v}{\partial t} \tag{2.56}$$

and

$$\frac{\partial^2 u}{\partial t^2} = \alpha^2 e^{\alpha t}v + 2e^{\alpha t}\frac{\partial v}{\partial t} + e^{\alpha t}\frac{\partial^2 v}{\partial t^2}. \tag{2.57}$$

so (2.57) becomes

$$\begin{aligned} &e^{\alpha t}\Delta v - cve^{\alpha t} \\ &= a\alpha e^{\alpha t}v + a\alpha e^{\alpha t}\frac{\partial v}{\partial t} + b\alpha^2 e^{\alpha t}v \\ &\quad + 2\alpha b\frac{\partial v}{\partial t} + be^{\alpha t}\frac{\partial^2 v}{\partial t^2} + f. \end{aligned} \tag{2.58}$$

Hence, letting $a + 2\alpha b = 0 \Rightarrow \alpha = -a/2b$ eliminates the first order derivatives in (2.58) and (2.58) takes the standard form

$$\Delta u - c'v = b\frac{\partial^2 v}{\partial t^2} + f' \tag{2.59}$$

for suitable c' and f'. We leave the details to the reader. Note that

$$c' = c + a^2/2b - a^2/4b^2 \tag{2.60}$$

which may be negative even if $c > 0$.

3 Conversion to the Modified Helmholtz Equation

As indicated in the Introduction, our approach to solving the time dependent equations (2.1) and (2.2) is to remove the time dependence and then solve the resulting elliptic equations. We will consider three methods for doing this; (i) the Laplace transform [Chen, Rashed and Golberg (1998)] (ii) finite differencing in time [Ingber

and Phan-Thien (1992); Chapko and Kress (1997)] (iii) the Laguerre transform [Chapko and Kress (2000)]. The application of these techniques to the IBVP for (2.5) or (2.6) reduces them to solving a sequence of inhomogeneous modified Helmholtz equations which can then be solved by a combination of the method of particular solutions (MPS) and Trefftz methods.

3.1 Parabolic Equations

3.1.1 The Laplace Transformation

Let $f(t)$ be a piece-wise continuous function of exponential growth on $[0,\infty)$. The Laplace transform $\hat{f}$ of f is defined by

$$\hat{f}(s) = \int_0^\infty e^{-st} f(t)\, dt. \tag{3.1}$$

To solve the IBVP for the diffusion equation, we take the Laplace transform of u giving $\hat{u}$ as the solution to

$$\Delta\hat{u}(P,s) - s\hat{u}(P,s) - c\hat{u}(P,s) = \hat{f}(P,s) - m(P) \tag{3.2}$$

where $u(P,0) = m(P)$. Defining $\lambda^2 = s + c$, $\hat{u}$ satisfies

$$\Delta\hat{u}(P,s) - \lambda^2\hat{u}(P,s) = v(P,s) \tag{3.3}$$

where $v(P,s) = \hat{f}(P,s) - m(P)$.

Similarly, taking the Laplace transform of the boundary condition gives

$$B\hat{u}(P,s) = \hat{g}(P,s) \tag{3.4}$$

where

$$\hat{g}(P,s) = \int_0^\infty e^{-st} g(P,t)\, dt \tag{3.5}$$

(where we have assumed that B is linear). Thus $\hat{u}(P,s)$ satisfies a BVP for the inhomogeneous modified Helmholtz equation (3.3) with boundary condition (3.4).

For numerical purposes one solves (3.3)-(3.4) for a sequence of values of $\{s_n\}_{n=1}^m$ and then applies a numerical inversion formula to the sequence $\{\hat{u}(P,s_n)\}_{n=1}^m$ [Stehfest (1970); Ganesh and Sheen (2001)]. Unfortunately, this can be problematic, as the numerical inversion of the Laplace transform is an ill-posed problem. Despite this, many inversion algorithms have appeared in the literature and an algorithm by [Stehfest (1970)] has found some success in the solution of diffusion problems. Recently, some work by [Ganesh and Sheen (2001)] has shown that it is possible to obtain a well-posed inversion algorithm, but it has yet to be implemented in conjunction with Trefftz methods. An interesting advantage of using the Laplace transform is that it leads to easily parallelizable algorithms, as the values $\{\hat{u}(P,s_n)\}_{n=1}^m$ can be obtained simultaneously by assigning the functions $\hat{u}(P,s_n)$ to individual processors.

3.1.2 Time Differencing

A variety of time differencing methods has been proposed to solve the IBVP for (2.5)-(2.6). Among these are, θ methods [Ingber, Chen and Tanski (2004); Ingber and Phan-Thien (1992)], time-splitting [Balakrishnan, Sureshkumar and Ramachandran (2002)] and methods based on A-stable multi-step methods for ordinary differential equations [Langdon (1999)]. As θ methods appear to be the most popular, we shall restrict our discussion to them.

For this, let $c > 0$ and define the mesh $t_n = n\tau$, $n \geq 0$. For $t_n \leq t \leq t_{n+1}$, approximate $u(P,t)$ by

$$u(P,t) \simeq \theta u(P,t_{n+1}) + (1-\theta)\, u(P,t_n), \tag{3.6}$$

and

$$\Delta u(P,t) \simeq \theta \Delta u(P,t_{n+1}) + (1-\theta)\, \Delta u(P,t_n), \tag{3.7}$$

where $0 < \theta \leq 1$ and

$$u_t(P,t) \simeq \frac{u(P,t_{n+1}) - u(P,t_n)}{\tau}. \tag{3.8}$$

Using (2.5)-(2.6) in Section 2 and denoting the resulting approximation to $u(P,t_n)$ by u_n, u_n satisfies

$$\begin{aligned}&\theta\Delta u_{n+1} + (1-\theta)\Delta u_n - c\left[\theta u_{n+1} + (1-\theta)u_n\right] \\ &= \frac{u_{n+1} - u_n}{\tau} + f_n\end{aligned} \tag{3.9}$$

where $f_n \equiv f(P,t_n)$. Rearranging (3.9) gives

$$\begin{aligned}&\Delta u_{n+1} - \frac{u_{n+1}}{\theta\tau} - cu_{n+1} \\ &= \frac{c(1-\theta)u_n}{\theta} - \frac{u_n}{\theta\tau} - \frac{(1-\theta)\Delta u_n}{\theta} + \frac{f_n}{\theta}.\end{aligned} \tag{3.10}$$

For $\theta = 1$ we get the backward Euler method

$$\Delta u_{n+1} - \frac{u_{n+1}}{\tau} - cu_{n+1} = -\frac{u_n}{\tau} + f_n. \tag{3.11}$$

Defining $\lambda^2 = c + 1/\tau$, (3.11) is of the form

$$\Delta u_{n+1} - \lambda^2 u_{n+1} = -\frac{u_n}{\tau} + f_n, \tag{3.12}$$

which is a sequence of inhomogeneous modified Helmholtz equations. From (2.9) we have the initial condition

$$u_0 = m(P) \tag{3.13}$$

and from (2.10) the boundary condition is

$$Bu_{n+1} = g_{n+1} = g(P,t_{n+1}), \tag{3.14}$$

so again numerically, the IBVP is reduced to solving a sequence of BVP for the inhomogeneous modified Helmholtz equation.

For $\theta = 0.5$ we get the Crank-Nicholson scheme

$$\begin{cases} \Delta u_{n+1} - \dfrac{2u_{n+1}}{\tau} - cu_{n+1} = cu_n - \dfrac{2u_n}{\tau} - \Delta u_n + 2f_n, \\ v_0 = m(P), \\ Bu_{n+1} = g_{n+1}. \end{cases} \tag{3.15}$$

Again, letting $\lambda^2 = c + 2/\tau$ $\{u_n\}$ satisfies a sequence of inhomogeneous modified Helmholtz equations.

Theoretically, one expects the Crank-Nicholson method to be more accurate than the backward Euler method, as the Euler approximation is $O(\tau)$ while the Crank-Nicholson method is $O\left(\tau^2\right)$. However, this improved accuracy may not be achieved in practice becuase of the loss in accuracy which occurs when u_n numerically evaluating the term Δu_n in the right hand side of Eq. (3.15).

It is interesting to note that one can apply time-differencing to the nonlinear diffusion equation

$$\Delta u = \frac{\partial u}{\partial t} + f(u). \tag{3.16}$$

For example, the backward Euler method gives

$$\Delta u_{n+1} - \frac{u_{n+1}}{\tau} = -\frac{u_n}{\tau} + f(u_n), \tag{3.17}$$

which again is a sequence of inhomogeneous modified Helmholtz equations. Numerical results for this equation can be found in [Golberg and Chen (2001)].

3.2 Hyperbolic Equations

3.2.1 The Laplace Transform

The IBVP for the wave equation is

$$\begin{cases} \Delta u - cu = \dfrac{\partial^2 u}{\partial t^2} + f,\ P \in D, \\ u(P,0) = m_1(P),\ u_t(P,0) = m_2(P), \\ Bu(P,t) = g(P,t),\ P \in S. \end{cases} \tag{3.18}$$

Taking the Laplace transform of (3.18) gives

$$\begin{aligned} &\Delta \hat{u}(P,s) - s^2 \hat{u}(P,s) - c\hat{u}(P,s) \\ &= -sm_1(P) + m_2(P),\ P \in D, \end{aligned} \tag{3.19}$$

and

$$B\hat{u}(P,s) = \hat{g}(P,s),\ P \in S. \tag{3.20}$$

As for the diffusion equation, (3.19)-(3.20) is solved for a sequence of values of $\{s_n\}_{n=1}^N$ and then applying a numerical inversion formula to $\{\hat{u}(P,s_n)\}_{n=1}^N$.

3.2.2 Time-differencing

Again we consider only the class of θ methods. For this again, defining $u_n(P) = u(P,t_n)$, we approximate

$$\frac{\partial^2 u}{\partial t^2} \simeq \frac{u_{n+1} - 2u_n + u_{n-1}}{\tau^2} \tag{3.21}$$

and

$$\Delta u(P,t) \simeq \theta \Delta u(P,t_{n+1}) + (1-\theta)\Delta u(P,t_n). \tag{3.22}$$

Again, letting u_n be the approximation to $u_n(P) \equiv u(P,t_n)$, and using (3.21)-(3.22) in (3.18), u_n satisfies

$$\begin{aligned} &\theta \Delta u_{n+1} + (1-\theta)\Delta u_n - c\left[\theta u_{n+1} + (1-\theta)u_n\right] \\ &= \frac{u_{n+1} - 2u_n + u_{n-1}}{\tau^2} + f_n \end{aligned} \tag{3.23}$$

and rearranging (3.23) gives

$$\begin{aligned} &\Delta u_{n+1} - \frac{u_{n+1}}{\theta\tau^2} - cu_{n+1} \\ &= \frac{c(1-\theta)u_n}{\theta} - \left(\frac{2u_n - u_{n-1}}{\theta\tau^2}\right) - \frac{(1-\theta)\Delta u_n}{\theta} + \frac{f_n}{\theta}. \end{aligned} \tag{3.24}$$

Now using the approximation

$$u_t \simeq \frac{u_{n+1} - u_n}{\tau} \tag{3.25}$$

we get the initial conditions

$$u_0(P) = m_1(P),\ P \in D \cup S \tag{3.26}$$

$$u_1(P) = m_1(P) + \tau m_2(P),\ P \in D \cup S \tag{3.27}$$

and the boundary conditions

$$Bw_{n+1}(P) = g_{n+1}(P),\ P \in S. \tag{3.28}$$

Hence, $\{u_n\}$ satisfies a BVP for an inhomogeneous modified Helmholtz equation as for the diffusion equation.

For $\theta = 0.5$ we obtain a second order Crank-Nicholson method.

3.3 The Laguerre Transform

Although time differencing is generally more reliable than the Laplace transform, it suffers from the problem of being unable to obtain high order accuracy and the overall convergence rate is usually limited by this property. Hence, it is desirable to have a transform method which does not suffer from the instability problem of the Laplace transform. A solution to this problem, the *Laguerre transform*, has recently been proposed by [Chapko and Kress (2000)] for use in conjunction with boundary integral methods. However, the method is applicable for use with Trefftz methods as we show next. We begin with the parabolic case.

We begin by defining the *normalized Laguerre polynomials* [Chapko and Kress (2000)].

$$L_n(r) = \frac{1}{n!} e^r \frac{d^n}{dr^n}\left(r^n e^{-r}\right),\ n = 0,1,2,... \tag{3.29}$$

It follows immediately that $\{L_n\}$ satisfy the recurrence relation

$$L'_{n+1} = L'_n - L_n \tag{3.30}$$

which in turn implies that

$$L'_n = -\sum_{m=0}^{n-1} L_m. \tag{3.31}$$

By Leibniz rule using (3.29) and (3.31), it follows that

$$L_n(0) = 1,\ L'_n(0) = -n,\ n \geq 0. \tag{3.32}$$

The Laguerre polynomials form a complete orthonormal system with respect to the inner product

$$\langle f, g\rangle = \int_0^\infty e^{-r} f(r) g(r)\, dr \tag{3.33}$$

in the space of real-valued functions in $L^2([0,\infty))$. Hence, any function f in $L^2([0,\infty))$ can be expanded in a series

$$f = \sum_{n=0}^{\infty} \langle f, L_a\rangle L_n. \tag{3.34}$$

Choosing a positive constant k, (3.34) can be scaled into the form

$$f(r) = k\sum_{n=0}^{\infty} f_n L_n(kr) \tag{3.35}$$

where

$$f_n = \int_0^\infty e^{-kr} L_n(r) f(r)\, dr. \tag{3.36}$$

For a bounded and continuously differentiable function f the Laguerre coefficients f'_n of the derivative f' are given by [Chapko and Kress (2000)]

$$f'_n = -f(0) + k\sum_{m=0}^{n} f_m,\ n \geq 0. \tag{3.37}$$

Also, the coefficients of the second derivative f'' are given by [Chapko and Kress (2000)]

$$f''_n = -f(0) + k(n+1) + k^2 \sum_{m=0}^{n} (n-m+1) f_m,\ n \geq 0. \tag{3.38}$$

Using (3.38), we obtain the following theorem.

Theorem 3.1 *Assume that $u(P,t)$ is a bounded, twice continuously differentiable solution to the diffusion equation* (3.18)*, with bounded first and second derivatives. Then the Laguerre coefficients of u*

$$u_n(P) = \int_0^\infty e^{-kt} L_n(kt)\, u(P,t)\, dt \tag{3.39}$$

satisfy the sequence of equations

$$\Delta u_n - c u_n = -m(P) + k\sum_{m=0}^{n} u_m + f_n,\ n \geq 0 \tag{3.40}$$

where

$$f_n = \int_0^\infty e^{-kt} L_n(kt)\, f(P,t)\, dt \tag{3.41}$$

and boundary conditions

$$Bu_n = g_n \tag{3.42}$$

where

$$g_n(P) = \int_0^\infty e^{-kt} L_n(kt)\, g(P,t)\, dt,\ n \geq 0. \tag{3.43}$$

Proof. Taking the Laguerre transform of both sides of (3.18) gives

$$\begin{aligned}&\int_0^\infty e^{-kt} L_n(kt)\left[\Delta u(P,t) - c u(P,t)\right] dt \\ &= \int_0^\infty e^{-kt} \frac{\partial u}{\partial t}(P,t) L_n(kt)\, dt + \int_0^\infty e^{-kt} f(P,t) L_n(kt)\, dt.\end{aligned} \tag{3.44}$$

Now by definition of the Laguerre coefficients and the differentiability of u, the left hand side of (3.44) becomes

$$\Delta u_n - c u_n. \tag{3.45}$$

From (3.37) the right hand side of (3.44) becomes

$$-u(P,0) + k\sum_{m=0}^{n} u_m + f_n. \tag{3.46}$$

It also follows from the initial condition that $u(P,0) = m(P)$ so that (3.46) becomes

$$-m(P) + k\sum_{m=0}^{n} u_m + f_n \tag{3.47}$$

and combining (3.45) and (3.47) gives (3.40).

For (3.39), take the Laguerre transform of the boundary condition $Bu = g$ to get (3.39).

Now rewriting (3.40) we see that u_n satisfy

$$\Delta u_n - c u_n - k u_u = k\sum_{m=0}^{n-1} u_m + f_n \equiv q_n \tag{3.48}$$

so that $\{u_n\}$ satisfies a sequence of inhomogeneous modified Helmholtz equations.

A drawback of this method is that it may be necessary to use fairly large numbers of terms ($n \geq 20$ [Chapko and Kress (2000)]) to get good convergence and this requires storing many terms to obtain the approximations. Further work is planned to determine the viability of this approach. Last, we note that in the Chapko-Kress paper they require zero initial values and zero source terms for their method to work. Also, their methodology seems, at present to be applicable only to problems in $\mathbb{R}^2$, whereas our methodology can be used both in $\mathbb{R}^2$ and $\mathbb{R}^3$.

For the hyperbolic case the Laguerre coefficients u_n of u can be shown to satisfy

$$\begin{aligned}&\Delta u_n - c u_n \\ &= \sum_{m=0}^{n} \beta_{n-m} u_m - m_2(P) \\ &\quad + [k(n+1)+1]\, m_1(P) + f_n(P)\end{aligned} \tag{3.49}$$

where

$$\beta_n = k^2(n+1) + k,\ n \geq 0 \tag{3.50}$$

with boundary conditions

$$Bu_n = g_n,\ n \geq 0. \tag{3.51}$$

This can be proved using (3.37) and (3.38). We leave the details to the reader.

4 The Trefftz Method

Until relatively recently, Trefftz methods had been limited to solving homogeneous linear elliptic equations. However, extensive research over the past decade on the numerical evaluation of particular solutions for elliptic operators has made it possible to extend this classical method to solve inhomogeneous elliptic, time-dependent and nonlinear equations. As we have seen, solving time-dependent PDEs requires solving a set of inhomogeneous Helmholtz equations. Hence, we consider boundary value problems for

$$Lu = \Delta u - \lambda^2 u = f. \tag{4.1}$$

To solve (4.1) by a Trefftz method, we begin by letting u_p be a particular solution to (4.1); i.e., u_p solves

$$Lu_p = f \tag{4.2}$$

but u_p does not necessarily satisfy the boundary conditions.

Then

$$v = u - u_p \tag{4.3}$$

satisfies

$$Lv = 0, \tag{4.4}$$

$$Bv = g - Bu_p. \tag{4.5}$$

Assuming u_p is known, we then need to solve (4.4)-(4.5).

In the Trefftz method, this is done as follows: we assume that $\{\nu_n\}_{n=0}^{\infty}$ is a complete basis of solutions to $Lv = 0$. That is, there exist constants $\{a_n\}_{n=0}^{N}$, such that

$$v_N = \sum_{n=0}^{N} a_n \nu_n \tag{4.6}$$

converges in norm to v. That is,

$$\left\| v - \sum_{n=0}^{N} a_n \nu_n \right\| \to 0,\ N \to \infty, \tag{4.7}$$

where $\|\cdot\|$ is a suitable norm on the solution set $\{Lv = 0\}$.

In this case, we try to determine

$$v_N = \sum_{n=0}^{N} a_n \nu_n \tag{4.8}$$

which provides a good approximation to the solution of the BVP. Since

$$Lv_N = 0, \tag{4.9}$$

we need only satisfy the boundary conditions. Since there is only a finite number of unknowns, we will not be able to satisfy the boundary condition exactly, but only approximately. Over the years, the following three primary methods have been proposed for doing this; (i) collocation, (ii) least squares, and (iii) Galerkin's method.

In collocation we choose N points $\left\{P_j\right\}_{j=1}^{N}$ on S and set

$$B\left(\sum_{k=1}^{N} a_k \nu_k\right)(P_j) = g(P_j) - Bu_p(P_j),\ 1 \le j \le N \tag{4.10}$$

which implies that

$$\sum_{k=1}^{N} a_k B\nu_k(P_j) = g(P_j) - Bu_p(P_j),\ 1 \le j \le N. \tag{4.11}$$

If (4.11) has a unique solution, then

$$u_N = v_N + u_p \tag{4.12}$$

is an approximate solution to the BVP

$$Lu(P) = f(P),\ P \in D, \tag{4.13}$$

$$Bu(P) = g(P),\ P \in S. \tag{4.14}$$

Unfortunately, little seems to be known theoretically about the solvability of (4.11) and the convergence of $\{u_N\}$ to u. Despite this, the collocation method has been used extensively during the past more than seventy years [Trefftz (1926)-Reutskiy (2002)]. In addition, the matrix

$$\mathbf{A}_c = \left[B\nu_k(P_j)\right],\ 1 \le j \le N, 1 \le k \le N \tag{4.15}$$

is generally ill-conditioned, so care must be taken when solving (4.11). We shall return to this matter later in Section 6.

In the method of least squares, one chooses $M \ge N$ points $\left\{P_j\right\}_{j=1}^{M}$ on S and defines

$$Q = \sum_{j=1}^{M} \left[Bv_N(P_j) - g(P_j) + Bu_p(P_j)\right]^2 \tag{4.16}$$

The coefficients $\{a_k\}_{k=1}^{N}$ in this case are chosen by minimizing Q with respect to $\{a_k\}_{k=1}^{N}$. Thus, differentiating Q with respect to $\{a_k\}_{k=1}^{N}$, these coefficients are obtained by solving

$$\frac{\partial Q}{\partial a_k} = 0,\ 1 \le k \le N, \tag{4.17}$$

giving $\mathbf{a} = (a_1, a_2, ..., a_N)^T$ as the solution to

$$\mathbf{A}_L^T \mathbf{A}_L \mathbf{a} = \mathbf{A}_L \mathbf{b} \tag{4.18}$$

where

$$\mathbf{A}_L = \left[B\nu_k(P_j)\right],\ 1 \le k \le N,\ 1 \le j \le M, \tag{4.19}$$

and

$$\mathbf{b} = [g(P_1) - Bu_p(P_1), g(P_2) - Bu_p(P_2), \cdots, g(P_M) - Bu_p(P_M)]^T. \tag{4.20}$$

A variant of this approach occurs when the basis functions ν_k depend on some additional parameters $\{\alpha_k\}_{k=1}^{l}$. Then the optimal values of $\{a_k\}_{k=1}^{N}$ and $\{\alpha_k\}_{k=1}^{l}$ are obtained by solving

$$\frac{\partial Q}{\partial a_k} = 0,\ 1 \le k \le N, \tag{4.21}$$

$$\frac{\partial Q}{\partial \alpha_k} = 0,\ 1 \le k \le l, \tag{4.22}$$

We will return to this in Section 6.1.

As for collocation, one expects the equations (4.18) to be ill-conditioned, so it is generally preferable to solve the minimization problem directly without solving the normal equations (4.18).

4.1 Galerkin's Method

In Galerkin's method [Bergman and Herriot (1961, 1965)], we choose some inner product $\langle \cdot, \cdot \rangle$ for functions on S and then set the residual

$$r_N = Bv_N - g + Bu_p \tag{4.23}$$

orthogonal to the basis elements $\{\nu_k\}_{k=1}^{N}$. In this case, $\{a_k\}_{k=1}^{N}$ are determined by solving

$$\langle Bv_N - g + Bu_p, \nu_k \rangle = 0,\ 1 \le k \le N. \tag{4.24}$$

To obtain an appropriate inner product, we use an argument analogous to that introduced by Bergman for solving Laplace's equation [Bergman and Herriot (1961)].

For $L=\Delta-c$, $c>0, Lu=0$ and $Lv=0$, we define

$$\langle u,v\rangle_D=\int_D\left[\sum_{i=1}^{d}\frac{\partial u}{\partial x_i}\frac{\partial v}{\partial x_i}+cuv\right]dV,\ d=2,3. \tag{4.25}$$

If X is the set of solutions to $Lv=0$, then $\langle u,v\rangle_D$ is an inner product on X.

Obviously, $\langle\cdot,\cdot\rangle_D$ is symmetric and bilinear and

$$\langle u,u\rangle_D=\int_D\left[\sum_{i=1}^{d}\left(\frac{\partial u}{\partial x_i}\right)^2+cu^2\right]dV\geq 0,\ d=2,3, \tag{4.26}$$

so $\langle u,u\rangle_D=0\Leftrightarrow u=0$. We now show that $\langle u,v\rangle_D$ is equivalent io an inner product on the boundary values of functions in X.

For this consider

$$div(u\text{grad}v)=div\left(u\frac{\partial v}{\partial x_1},u\frac{\partial v}{\partial x_2},u\frac{\partial v}{\partial x_3}\right),\ \text{in}\ \mathbb{R}^3 \tag{4.27}$$

and

$$div(u\text{grad}v)=div\left(u\frac{\partial v}{\partial x_1},u\frac{\partial v}{\partial x_1}\right),\ \text{in}\ \mathbb{R}^2 \tag{4.28}$$

Now,

$$\begin{aligned}&div(u\text{grad}v)\\&=\frac{\partial}{\partial x_1}\left(u\frac{\partial v}{\partial x_1}\right)+\frac{\partial}{\partial x_2}\left(u\frac{\partial v}{\partial x_2}\right)+\frac{\partial}{\partial x_3}\left(u\frac{\partial v}{\partial x_3}\right)\\&=\sum_{i=1}^{3}\frac{\partial u}{\partial x_i}\left(\frac{\partial v}{\partial x_i}\right)+u\Delta v,\ \text{in}\ \mathbb{R}^3\end{aligned} \tag{4.29}$$

and

$$div(u\text{grad}v)=\sum_{i=1}^{2}\frac{\partial u}{\partial x_i}\left(\frac{\partial v}{\partial x_i}\right)+u\Delta v,\ \text{in}\ \mathbb{R}^2. \tag{4.30}$$

Since $\Delta v=cv$,

$$div(u\text{grad}v)=\sum_{i=1}^{d}\frac{\partial u}{\partial x_i}\left(\frac{\partial v}{\partial x_i}\right)+cuv,\ d=2,3 \tag{4.31}$$

so

$$\langle u,v\rangle_D=\int_D div(u\text{grad}v)\,dV. \tag{4.32}$$

By the divergence theorem,

$$\int_D div(u\text{grad}v)\,dV=\int_S(u\text{grad}v)\cdot\mathbf{n}dS \tag{4.33}$$

where $\mathbf{n}$ is the unit outward normal on S. But

$$\text{grad}v\cdot\mathbf{n}=\frac{\partial v}{\partial\mathbf{n}} \tag{4.34}$$

is the normal derivative of v. Hence, it follows from (4.32) and (4.33) that

$$\langle u,v\rangle_D=\int_S u\frac{\partial v}{\partial\mathbf{n}}dS\equiv\langle u,v\rangle_S \tag{4.35}$$

Similarly,

$$\langle u,v\rangle_S=\int_S v\frac{\partial u}{\partial\mathbf{n}}dS. \tag{4.36}$$

It now follows from the fact that $\langle u,v\rangle_D$ is an inner product that $\langle\cdot,\cdot\rangle_S$ is an inner product on the boundary values of functions in X.

Using this inner product, (4.24) becomes

$$\langle Bv_N-g+Bu_p,\nu_k\rangle_S=0,\ 1\leq k\leq N. \tag{4.37}$$

Since $v_N=\sum_{j=1}^{N}a_jB\nu_j$, (4.37) gives

$$\sum_{j=1}^{N}a_jB\left\langle\nu_j,\nu_k\right\rangle_S=\langle g-Bu_p,\nu_k\rangle_S,\ 1\leq k\leq N. \tag{4.38}$$

Now suppose that we have Dirichlet boundary conditions on u, then, $Bv_N=v_N$ so (4.38) becomes

$$\sum_{j=1}^{N}a_j\left\langle\nu_j,\nu_k\right\rangle_S=\langle g-Bu_p,\nu_k\rangle_S,\ 1\leq k\leq N. \tag{4.39}$$

If $\left\{\nu_j\right\}_{j=1}^{\infty}$ are linearly independent, then the matrix

$$\mathbf{A}_G=\left[\left\langle\nu_j,\nu_k\right\rangle\right],\ 1\leq j,k\leq N \tag{4.40}$$

is a Gram matrix. Hence, it is positive definite, and so it is invertible.

For Neumann boundary conditions, $Bu=\partial u/\partial\mathbf{n}$ and in this case

$$\left\langle B\nu_j,\nu_k\right\rangle_S=\int_S\frac{\partial\nu_j}{\partial\mathbf{n}}\frac{\partial\nu_k}{\partial\mathbf{n}}ds \tag{4.41}$$

so this matrix will be invertible provided the derivatives $\left\{\partial\nu_j/\partial\mathbf{n}\right\}_{j=1}^{N}$ are linearly independent. Similarly, we can establish invertability for Robin boundary conditions provided $\alpha(P)>0, P\in S$.

As a consequence, the Galerkin equations (4.24) have a unique solution, in contrast to collocation and least squares, where no such theorem is known.

A further observation is that, if the bases are chosen so that $\left[\left\langle B\nu_j,\nu_k\right\rangle\right]$ is the identity matrix, then obviously it will not be ill-conditioned. Generally, we expect Galerkin's method to be better conditioned than either collocation or least squares.

Although Galerkin's method appears to have better theoretical properties than either collocation or least squares, there are some problems in its implementation because of the need to evaluate the integrals $\left\langle B\nu_j,\nu_k\right\rangle_S$ and $\left\langle g-Bu_p,\nu_k\right\rangle_S, 1\le j,k\le N$.

In $\mathbb{R}^2$, if S is a smooth closed curve, this generally can be done by using the trapezoidal rule, which was done by Bergman in [Bergman and Herriot (1961)].

However, if S is a surface in $\mathbb{R}^3$, this is a much more difficult problem. If S has a simple shape, such as a sphere or a cube, then standard integration rules can be used to do this efficiently [Golberg and Chen (1996); Stroud (1971)]. More generally, if S can be decomposed into a finite union of simple shapes, then the integrals can be decomposed into a finite sum of standard integrals. More generally, this may have to be done by a triangulation scheme as used in the BEM [Golberg and Chen (1996)]. However, the resulting method should still be less computationally complex than the BEM, since all integrals are non-singular.

5 Particular Solutions

Over the past 20 years extensive research has been done on the numerical evaluation of particular solutions of elliptic operators spurred by the work of [Nardini and Brebbia (1982)], [Mayo (1984, 1992)], [McKenney, Greengard and Mayo (1995)], and [Atkinson (1985)]. In general, these methods fall into two distinct classes, direct methods which approximate a solution to $Lu_p = f$ by some numerical method, and the indirect approach found in the Dual Reciprocity Method (DRM) [Partridge, Brebbia and Wrobel (1992); Nardini and Brebbia (1982)].

In the DRM the source term f in $\Delta u_p - \lambda^2 u_p = f$ is approximated as

$$f \simeq \hat{f} = \sum_{k=1}^{N} a_k \varphi_k \tag{5.1}$$

where $\{\varphi_k\}_{k=1}^N$ is an appropriate set of basis functions. Then we define

$$\hat{u}_p = \sum_{k=1}^{N} a_k \psi_k \tag{5.2}$$

where $\{\psi_k\}_{k=1}^N$ solve

$$\Delta\psi_k - \lambda^2\psi_k = \varphi_k. \tag{5.3}$$

Generally, it is best to have analytic expressions for ψ_k. By linearity,

$$\Delta\hat{u}_p = \hat{f}, \tag{5.4}$$

so we may regard $\hat{u}_p$ as an approximate particular solution. Note that in this approach $\hat{u}_p$ generally does not approximate an exact particular solution of $\Delta u_p - \lambda^2 u_p = f$ [Golberg, Chen, Bowman and Power (1998)].

We begin our discussion by considering some direct approaches and then develop the DRM approach in detail.

5.1 Numerical Integration

As is well known, a particular solution of $\Delta u_p - \lambda^2 u_p = f$ is given by [Partridge, Brebbia and Wrobel (1992)]

$$u_p(P) = \int_D G(P,Q;\lambda)\, f(Q)\, dV \tag{5.5}$$

where $G(P,Q;\lambda)$ is the fundamental solution of the operator $\Delta - \lambda^2$, and $G(P,Q;\lambda)$ is a solution to

$$\Delta G(P,Q;\lambda) - \lambda^2 G(P,Q;\lambda) = \delta(P-Q) \tag{5.6}$$

where $\delta(P-Q)$ is the Dirac delta function. It is known that

$$G(P,Q;\lambda) = \frac{1}{2\pi} K_0(\lambda r), \text{ in } \mathbb{R}^2, \tag{5.7}$$

and

$$G(P,Q;\lambda) = \frac{1}{4\pi}\frac{\exp(-\lambda r)}{r}, \text{ in } \mathbb{R}^3, \tag{5.8}$$

where $r = \|P-Q\|$ is the Euclidean distance between P and Q and K_0 is the Bessel function of the third kind of order zero.

In general, the integral in (5.5) cannot be evaluated analytically and some form of numerical integration needs to be used. This is not straightforward since $G(P,Q;\lambda)$ is singular and D can have an arbitrary shape. This generally requires a finite element approach where D is decomposed into triangles in $\mathbb{R}^2$ and tetrahedra in $\mathbb{R}^3$. Then the

integral is approximated by a sum of integrals over each element. If D is simply connected, then one can use a fanning decomposition as shown in Figure 5.1 [Partridge, Brebbia and Wrobel (1992)].

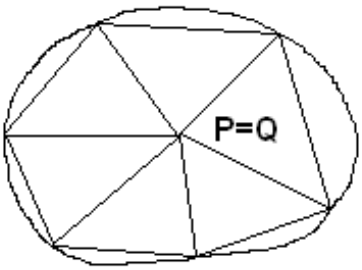

Figure 5.1: Fanning decomposition

In this approach the elements are centered at the singular point $P = Q$ and then polar coordinates are introduced in each element to weaken the singularity. If D is multiply connected, a more complex approach must be used.

In the BEM this technique has been assumed to be more complex than the DRM approach. However, some recent work by [Ingber, Mammoli and Brown (2001)] combines numerical integration with multipole acceleration to obtain a more efficient version of this technique. Some numerical experiments indicate that it may be more efficient than the DRM under certain circumstances. However, the accuracy of the method is limited by the accuracy of the boundary approximation needed to do the numerical integration which is generally not of high order. Since Trefftz methods are generally spectrally convergent for smooth data, this method may not be suitable for use with these methods.

5.2 Atkinson's Method

A somewhat simpler numerical integration method was proposed by [Atkinson (1985)] for Poisson's equation but can be easily extended to Helmholtz-type equations.

In this method we assume that the source term f can be extended smoothly outside of the domain D to a domain $\hat{D} \supseteq D$. Then

$$u_p(P) = \int_{\hat{D}} G(P,Q;\lambda)\, f(Q)\, dV \tag{5.9}$$

is also a particular solution of $\Delta u_p - \lambda^2 u_p = f$. If $\hat{D}$ is chosen as an ellipse in $\mathbb{R}^2$ or an ellipsoid in $\mathbb{R}^3$, then a simple coordinate transformation converts (5.9) to a form which can be evaluated by standard numerical integration rules.

5.3 The DRM

In the DRM a variety of bases can be used to approximate the sources terms. Among these are: radial basis functions (RBFs), [Golberg, Muleshkov, Chen and Cheng (2003); Muleshkov, Golberg and Chen (1999); Golberg, Chen and Ganesh (2000); Chen, Golberg, Ganesh and Cheng (2002)] polynomials or trigonometric functions [Li and Chen (2004)], and a number of numerical methods can be used, such as interpolation, least squares or approximation methods. In this paper, we focus on interpolation and approximation methods [Li and Chen (2004)].

To use polynomial or trigonometric bases, we need to be able to extend f smoothly to a domain $\hat{D} \supseteq D$ as in Atkinson's method. For RBFs no such extension is necessary. We begin with this approach.

Definition 5.1 Let $\varphi : [0,\infty) \to \mathbb{R}$ be a continuous function. Let $\{P_j\}_{j=1}^N$ be N distinct points in $\mathbb{R}^d, d = 2,3$. A function of the form

$$f(P) = \sum_{j=1}^{N} a_j \varphi\left(\left\|P - P_j\right\|\right) + p_m(P) \tag{5.10}$$

where $\|\cdot\|$ is the Euclidean norm on $\mathbb{R}^d$ and p_m is a polynomial of degree m is called a *radial basis function* (RBF).

As indicated previously, to use RBFs to find particular solutions we approximate f by a RBF and then we obtain an approximate particular solution as

$$\hat{u}_p(P) = \sum_{j=1}^{N} a_j \psi_j(P) + \chi_m(P) \tag{5.11}$$

where

$$\Delta\psi_j - \lambda^2\psi_j = \varphi_j(P),\ \varphi_j(P) = \varphi\left(\left\|P - P_j\right\|\right) \tag{5.12}$$

and

$$\Delta\chi_m - \lambda^2\chi_m = p_m. \tag{5.13}$$

Because it is generally more efficient numerically to solve (5.12)-(5.13) analytically, this limits the choice of RBFs one can use. In $\mathbb{R}^2$, one can use thin plate and polyharmonic splines [Muleshkov, Golberg and Chen (1999)], while in $\mathbb{R}^3$ one can use splines and Wendland's

compactly supported radial basis functions (CS-RBFs) [Wenland (1995)]. It is also possible to use inverse multiquadrics and Gaussians. We begin with splines.

In $\mathbb{R}^2$ a spline is of the form [Duchon (1976, 1978); Powell (1992)]

$$\varphi^{[n]}(r) = r^{2n}\log r,\ n \geq 1 \tag{5.14}$$

and p_m is a polynomial of degree $m = n$. For $n = 1$ these are the *thin plate splines* (TPS)

$$\varphi^{[1]}(r) = r^2 \log r \tag{5.15}$$

and

$$p_1 = ax + by + c. \tag{5.16}$$

In $\mathbb{R}^3$ the splines are of the form [Duchon (1976)]

$$\varphi^{[n]}(r) = r^{2n-1},\ n \geq 1, \tag{5.17}$$

and p_m is a polynomial with $m = n$. For $n = 1$, these are the TPS

$$\varphi^{[1]}(r) = r \tag{5.18}$$

with

$$p_1 = ax + by + cz + d. \tag{5.19}$$

The importance of splines is that they can provide interpolatory approximations to f for very general sets of interpolation points $\left\{P_j\right\}_{j=1}^N$ in $\mathbb{R}^d$. For example, in $\mathbb{R}^2$ if $\left\{P_j\right\}_{j=1}^N$ are not collinear, then there is a unique solution $\left\{\left\{a_j\right\}_{j=1}^N, a, b, c\right\}$ satisfying the interpolation conditions

$$\sum_{j=1}^N a_j \left\|P_j - P_k\right\|^2 \log\left(\left\|P_j - P_k\right\|\right) + ax_k + by_k + c$$
$$= f(P_k),\ 1 \leq k \leq N, \tag{5.20}$$

and

$$\sum_{j=1}^N a_j = \sum_{j=1}^N a_j x_j = \sum_{j=1}^N a_j y_j = 0, \tag{5.21}$$

where $P_k = (x_k, y_k)$, $1 \leq k \leq N$.

In $\mathbb{R}^3$, if $\left\{P_j\right\}_{j=1}^N$ are not coplanar, then there is a unique solution $\left\{\left\{a_j\right\}_{j=1}^N, a, b, c, d\right\}$ to the equations

$$\sum_{j=1}^N a_j \left(\left\|P_j - P_k\right\|\right) + ax_k + by_k + cz_k + d$$
$$= f(P_k),\ 1 \leq k \leq N, \tag{5.22}$$

and

$$\sum_{j=1}^N a_j = \sum_{j=1}^N a_j x_j = \sum_{j=1}^N a_j y_j = \sum_{j=1}^N a_j z_j = 0, \tag{5.23}$$

where $P_k = (x_k, y_k, z_k)$, $1 \leq k \leq N$.

In addition, the TPS are optimal interpolants in the sense that they minimize the semi-norm [Duchon (1976)]

$$\int_{\mathbb{R}^d} \sum_{j=1}^d \left(\frac{\partial^2 f}{\partial x_j^2}\right)^2 dV,\ d = 2, 3. \tag{5.24}$$

For higher order splines we assume that $\left\{P_j\right\}_{j=1}^N$ is a insolvent set of points for polynomial interpolation and let $\{b_k\}_{k=1}^{l_n}$ be a basis for P_n, the set of polynomials of degree $\leq n$ ($l_n = \binom{n+d}{d}$, $d = 2, 3$ is the dimension of P_n). Then there is a unique solution to the interpolation equations

$$\sum_{j=1}^N a_j \varphi^{[n]}\left(\left\|P_j - P_k\right\|\right) + p_n(P_k) = f(P_k), 1 \leq k \leq N, \tag{5.25}$$

and

$$\sum_{j=1}^N a_j b_l(P_j) = 0,\ 1 \leq l \leq l_n. \tag{5.26}$$

In general, the accuracy of the spline approximation increases as the order n of the spline increases and the number N of interpolation points increases. In fact, if $\|\cdot\|_2$ denotes the L^2 norm of functions on D, it is known that [Duchon (1978)]

$$\left\|f - \hat{f}\right\|_2 \leq ch^n \tag{5.27}$$

where

$$h = \sup_{P \in \mathbb{R}^d} \min_{Q \in \left\{P_j\right\}} \|P - Q\| \tag{5.28}$$

is the 'mesh width' of the points $\left\{P_j\right\}_{j=1}^N$ and c is a constant independent of h.

However, as n increases and h decreases the matrix $\mathbf{A}$ of the linear system (5.25)-(5.26) becomes more ill-conditioned. In fact it follows from [Li and Golberg (2003); Schaback (1995)] that

$$cond(\mathbf{A}) \simeq ch^{-n} \tag{5.29}$$

where again c does not depend on h. Hence, finding the appropriate trade-off between the order of spline and the number of interpolation points is not obvious. As can be seen from Table 5.1 the complexity of the particular solution increases as the order n increases so generally we have found that it is preferable to use splines of moderate order. In our work, $n \leq 4$ has given good results [Muleshkov, Golberg and Chen (1999)]. Increasing the number of interpolation points can then be used to increase the accuracy of the interpolation [Duchon (1978); Schaback (1995)]. Some authors have also found that increasing the degree of polynomial $m > n$ in (5.25) can also improve the accuracy of the approximation [Ingber, Chen and Tanski (2004)].

Having obtained the spline approximation $\hat{f}$ to f we now consider finding the particular solutions $\psi_j, 1 \leq j \leq N$ and χ_n. For ψ_j we use the fact that φ_j is the fundamental solution of the iterated Laplacian Δ^n. That is,

$$\Delta^n \varphi_j^{[n]} = \delta(P - P_j). \tag{5.30}$$

Hence, applying Δ^n to (5.12), we find that ψ_j satisfies

$$\Delta^n \left(\Delta - \lambda^2\right) \psi_j = 0,\ P \neq P_j,\ 1 \leq j \leq N. \tag{5.31}$$

Since $\varphi_j^{[n]}$ is radially symmetric, ψ_j can be chosen to be radially symmetric as well. Hence, defining $\psi(r)$ as the solution to

$$\Delta_r^n \left(\Delta_r - \lambda^2\right) \psi = 0,\ r > 0, \tag{5.32}$$

where Δ_r is the radial part of the Laplacian Δ, i.e.,

$$\Delta_r u = \frac{1}{r}\frac{d}{dr}\left(\frac{rdu}{dr}\right), \text{ in } \mathbb{R}^2, \tag{5.33}$$

and

$$\Delta_r u = \frac{1}{r^2}\frac{d}{dr}\left(\frac{r^2 du}{dr}\right), \text{ in } \mathbb{R}^3, \tag{5.34}$$

then

$$\psi_j = \psi\left(\left\|P - P_j\right\|\right),\ 1 \leq j \leq N. \tag{5.35}$$

Note that (5.32) is a $(2n+2)$-th order ordinary differential equation. Since Δ_r and $\Delta_r - \lambda^2$ commute, it follows that

$$\psi = u + v \tag{5.36}$$

where

$$\Delta_r^2 u - \lambda^2 u = 0, \tag{5.37}$$

and

$$\Delta_r^n v = 0. \tag{5.38}$$

Using the fact that $\Delta_r - \lambda^2$ is a Bessel operator and Δ_r^n is essentially an Euler operator [Derrick and Grossman (1976)], it was shown in [Muleshkov, Golberg and Chen (1999)] that

$$\begin{aligned}&\psi(r)\\ &= AI_0(\lambda r) + BK_0(\lambda r) + \sum_{k=1}^{n+1} c_k r^{2k-2}\log r + \sum_{k=1}^{n+1} d_k r^{2k-2}\end{aligned} \tag{5.39}$$

where

$$B = -\frac{\left[(2n)!!\right]^2}{\lambda^{2n+2}}, \tag{5.40}$$

$$c_k = -\frac{\left[(2n)!!\right]^2}{\left[(2k-2)!!\right]^2}\lambda^{2k-2n-4},\ 1 \leq k \leq n+1, \tag{5.41}$$

$$d_k = c_k \sum_{j=k}^{n}\left(\frac{1}{j}\right),\ 1 \leq k \leq n, \text{ in } \mathbb{R}^2, \tag{5.42}$$

where I_0 and K_0 are Bessel functions of the second and third kinds of order zero respectively, and

$$(2k)!! = 2 \times 4 \times 6 \times \cdots \times 2k,\ k \geq 1.$$

Also,

$$\begin{aligned}&\psi(r)\\ &= \frac{(-1)^{n+1}(2n)!}{r\lambda^{2n+2}}\cosh(\lambda r) + \sum_{k=0}^{n}\frac{(2n)!}{(2k)!}\frac{r^{2k-1}}{\lambda^{2n-2k+2}},\end{aligned} \tag{5.43}$$

in $\mathbb{R}^3$.

Since A is arbitrary in (5.39), we choose it to be zero. Moreover, for computational purposes, it is more convenient to use the forms

$$\begin{aligned}&\psi(r)\\ &= B\sum_{k=0}^{\infty} c_k r^{2k} - B\sum_{k=n+1}^{\infty}\frac{\lambda^{2k}}{\left[(2k)!!\right]^2}r^{2k}\log r + \sum_{k=1}^{n+1} d_k r^{2k-2}\end{aligned} \tag{5.44}$$

in $\mathbb{R}^2$ and

$$\psi(r) = \sum_{k=n+1}^{\infty} \frac{(2n+1)!}{(2k+1)!} \frac{r^{2k}}{\lambda^{2n-2k+2}}, \text{ in } \mathbb{R}^3. \tag{5.45}$$

These expressions show that ψ is C^{2n+1} in $\mathbb{R}^2$ and analytic in $\mathbb{R}^3$.

To find χ_n the most straightforward way is to decompose p_n as

$$p_n = \sum_{k=0}^{n} a_k x^n y^{n-k}, \text{ in } \mathbb{R}^2 \tag{5.46}$$

and

$$p_n = \sum_{0 \le k+m+p \le n} a_{k,m,p} x^k y^m z^p, \text{ in } \mathbb{R}^3 \tag{5.47}$$

and then finding the solution b_k to

$$\left(\Delta^2 - \lambda^2\right) b_k = x^k y^{n-k}, \ 0 \le k \le n \tag{5.48}$$

in $\mathbb{R}^2$ and

$$\left(\Delta^2 - \lambda^2\right) b_{k,m,p} = x^k y^m z^p, \ 0 \le k+m+p \le n \tag{5.49}$$

in $\mathbb{R}^2$. This can be done by the method of undetermined coefficients [Golberg, Muleshkov, Chen and Cheng (2003); Muleshkov, Chen, Golberg and Cheng (2000)], and an explicit solution will be given in Section 5.6. In [Muleshkov, Golberg and Chen (1999)] another formula was given without proof. Because this approach can be generalized to other operators, we give a derivation here.

Suppose now that p is a polynomial of degree m and consider solving

$$Lu_p - \lambda^2 u_p = p \tag{5.50}$$

where L is a linear differential operator with constant coefficients. From (5.50)

$$\left(L - \lambda^2 I\right) u_p = p \tag{5.51}$$

where I is the identity operator. Then formally,

$$u_p = \left(L - \lambda^2 I\right)^{-1} p = -\frac{1}{\lambda^2} \left(I - \frac{L}{\lambda^2}\right)^{-1} p. \tag{5.52}$$

Expanding $\left(I - L/\lambda^2\right)^{-1}$ in a geometric series gives

$$\left(I - \frac{L}{\lambda^2}\right)^{-1} = \sum_{k=0}^{n} \left(\frac{L}{\lambda^2}\right)^k \tag{5.53}$$

so that

$$u_p = -\frac{1}{\lambda^2} \sum_{k=0}^{\infty} \frac{L^k p}{\lambda^{2k}}. \tag{5.54}$$

Since p is a polynomial of degree m, there exists an integer j such that $L^k p = 0, k > j$. Thus,

$$u_p = -\frac{1}{\lambda^2} \sum_{k=0}^{j} \frac{L^k p}{\lambda^{2k}} \tag{5.55}$$

is well defined and can easily be shown to satisfy $Lu_p - \lambda^2 u_p = p$. Letting $L = \Delta$,

$$u_p = -\sum_{k=0}^{j} \frac{\Delta^k p}{\lambda^{2k+2}} \tag{5.56}$$

is a particular solution for $\Delta u_p - \lambda^2 u_p = p$. This formula agrees with the one given in [Muleshkov, Golberg and Chen (1999)].

As an example suppose φ is a TPS, then $p = p_1$ and (5.56) gives

$$u_p = -p_1/\lambda^2 \tag{5.57}$$

since $\Delta^k p_1 = 0, k \ge 1$.

5.4 Kansa's Method

As can be seen from Table 5.1, the particular solutions become increasingly complex as the order of splines increases. As a consequence, it is interesting to consider other techniques that may be less analytically complicated. One way of doing this is to use Kansa's method [Kansa (1990a, 1990b)]. Here, we proceed as follows.

Let ψ_j be a RBF and define

$$\varphi_j = L\psi_j. \tag{5.58}$$

Now approximate f by $\varphi_j, 1 \le j \le N$. Then

$$f \simeq \hat{f} = \sum_{j=1}^{N} a_j \varphi_j \tag{5.59}$$

where $\hat{f}$ can be obtained by interpolation as for splines. Define

$$\hat{u}_p = \sum_{j=1}^{N} a_j \psi_j \tag{5.60}$$

Table 5.1 Particular Solutions and the Values of Order n

φ	Ψ
$r^2\log r$	$\begin{cases} -\frac{4}{\lambda^4}\left[K_0(\lambda r)+\log r\right]-\frac{r^2\log r}{\lambda^2}-\frac{4}{\lambda^4}, & r>0 \\ \frac{4}{\lambda^4}\left[\gamma+\log(\lambda/2)\right]-\frac{4}{\lambda^4}, & r=0 \end{cases}$
$r^4\log r$	$\begin{cases} -\frac{64}{\lambda^6}\left[K_0(\lambda r)+\log r\right]-\frac{r^2\log r}{\lambda^2}\left(\frac{16}{\lambda^2}+r^2\right)-\frac{8r^2}{\lambda^4}-\frac{96}{\lambda^6}, & r>0 \\ \frac{64}{\lambda^6}\left[\gamma+\log(\lambda/2)\right]-\frac{96}{\lambda^6}, & r=0 \end{cases}$
$r^6\log r$	$\begin{cases} -\frac{2304}{\lambda^8}\left[K_0(\lambda r)+\log r\right]-\frac{r^2\log r}{\lambda^2}\left(\frac{576}{\lambda^4}+\frac{36r^2}{\lambda^2}+r^4\right) \\ -\frac{12r^2}{\lambda^4}\left(\frac{40}{\lambda^2}-r^2\right)-\frac{4224}{\lambda^8}, \quad r>0 \\ \frac{2304}{\lambda^8}\left[\gamma+\log(\lambda/2)\right]-\frac{4224}{\lambda^8}, \quad r=0 \end{cases}$
$r^8\log r$	$\begin{cases} -\frac{147456}{\lambda^{10}}\left[K_0(\lambda r)+\log r\right]-\frac{r^2\log r}{\lambda^2}\left(\frac{36864}{\lambda^6}+\frac{2304r^2}{\lambda^4}+\frac{64r^4}{\lambda^2}\right) \\ -\frac{r^2}{\lambda^4}\left(\frac{39936}{\lambda^4}+\frac{1344r^2}{\lambda^2}-16r^4\right)-\frac{307200}{\lambda^{10}}, \quad r>0 \\ \frac{147456}{\lambda^{10}}\left[\gamma+\log(\lambda/2)\right]-\frac{307200}{\lambda^{10}}, \quad r=0 \end{cases}$
$r^{10}\log r$	$\begin{cases} -\frac{14745600}{\lambda^{12}}\left[K_0(\lambda r)+\log r\right]-\frac{r^2\log r}{\lambda^2}\left(\frac{3686400}{\lambda^8}+\frac{230400r^2}{\lambda^6}\right. \\ \left.+\frac{6400r^4}{\lambda^4}+r^6\right)-\frac{r^2}{\lambda^4}\left(\frac{4730880}{\lambda^6}+\frac{180480r^2}{\lambda^4}+\frac{2880r^2}{\lambda^2}+20r^6\right) \\ -\frac{33669120}{\lambda^{12}}, \quad r>0 \\ \frac{14745600}{\lambda^{12}}\left[\gamma+\log(\lambda/2)\right]-\frac{33669120}{\lambda^{12}}, \quad r=0 \end{cases}$

In Table 5.1, $\gamma\simeq 0.5772156649015328$, which is known as Euler's constant.

then,

$$L\hat{u}_p=\sum_{j=1}^{N}a_jL\psi_j=\sum_{j=1}^{N}a_j\varphi_j=\hat{f}. \tag{5.61}$$

So, $\hat{u}_p$ is an approximate particular solution to $Lu_p=f$.

For this method to be mathematically correct, it is necessary that the interpolation problem

$$\sum_{j=1}^{N}a_j\varphi_j(P_k)=f(P_k),\ 1\le k\le N \tag{5.62}$$

be uniquely solvable. Unfortunately, a number of authors have used this approach without guaranteeing this property. However, there is a number of cases where this can be proved, in particular, when φ is a positive definite RBF.

Definition 5.2 Let φ be a RBF. We say that φ is positive definite if and only if for every subset of points $\left\{P_j\right\}_{j=1}^{N}$ in $\mathbb{R}^d$ the matrices

$$\mathbf{A}_\varphi=\left[\varphi\left(\left\|P_k-P_j\right\|\right)\right],\ 1\le j,k\le N, \tag{5.63}$$

are positive definite in the usual sense in linear algebra.

Since positive definite matrices are invertible, the interpolation equations (5.58) will have a unique solution. Now, if ψ is a positive definite RBF, it follows from Bochner's theorem [Bochner (1959)] and the fact that $\Delta-\lambda^2$ is a negative definite operator that $\varphi=L\psi$ is a negative definite RBF. In this case, the interpolation matrix in (5.63) is negative definite, so again the interpolation problem has a unique solution. Fortunately, there is a number of well known positive definite RBFs. Among

these are, the *inverse multiquadratics* (IMQs)

$$\varphi(r) = \left(r^2 + c^2\right)^{-1/2} \tag{5.64}$$

and *Gaussians*

$$\psi(r) = \exp\left(-cr^2\right) \tag{5.65}$$

and Wendland's CS-RBFs to be discussed in the following section.

One drawback to this approach is that, to the best of our knowledge, the approximation properties of $\varphi = \left(\Delta - \lambda^2\right)\psi$ appear not to be known. However, for IMQs and Gaussians, we expect rapid convergence, if f is smooth.

5.5 Compactly Supported RBFs

Since splines, IMQs, and Gaussians are globally supported, the linear systems of equations needed for interpolation are dense and can be quite large and ill-conditioned, particularly for problems in $\mathbb{R}^3$. As a consequence, for many years, the 'holy grail' of the RBF community was to find a class of compactly supported RBFs (CS-RBFs) for which the interpolation problem was uniquely solvable. This problem was first solved in the mid-1990's by [Wu (1995)] and [Wenland (1995)]. For our purposes, we concentrate on Wendland's CS-RBFs. They are of the form

$$\varphi(r) = \begin{cases} (1-r)_+^n p(r), & 0 \le r \le 1, \\ 0, & r > 1, \end{cases} \tag{5.66}$$

where

$$(1-r)_+ = \begin{cases} 1-r, & 0 \le r \le 1, \\ 0, & r > 1. \end{cases} \tag{5.67}$$

and $p(r)$ is a polynomial of suitable degree.

In $\mathbb{R}^d$, $d = 2, 3$, the first four CS-RBFs are

$$\varphi_1(r) = (1-r)_+^2, \tag{5.68}$$

$$\varphi_2(r) = (1-r)_+^4 (4r+1), \tag{5.69}$$

$$\varphi_3(r) = (1-r)_+^6 \left(35r^2 + 18r + 3\right), \tag{5.70}$$

and

$$\varphi_4(r) = (1-r)_+^8 \left(32r^3 + 25r^2 + 8r + 1\right). \tag{5.71}$$

Since Wendland's CS-RBFs are positive definite, the interpolation problem is uniquely solvable for arbitrary sets of interpolation points $\left\{P_j\right\}_{j=1}^N$.

For efficient interpolation, it is necessary to consider the scaled RBFs

$$\varphi_a(r) = (1 - r/a)_+^n p(r/a) \tag{5.72}$$

with support in $[0, a]$ rather than $[0, 1]$. For a given set of interpolation points, the interpolation matrices $\mathbf{A}_\varphi$ are sparse with the sparseness increasing as a decreases. On the other hand, the approximation accuracy increases as a increases. Hence, it is important to find the optimal trade-off between sparsity and accuracy. At present, the best approach to this problem seems to be the use of multilevel methods as discussed in [Golberg, Chen and Ganesh (2000); Chen, Golberg, Ganesh and Cheng (2002); Floater and Iske (1996)]. We refer the reader there for details.

To compute particular solutions to $\left(\Delta - \lambda^2\right) u_p = \varphi$ two methods have been discussed, Kansa's method in $\mathbb{R}^2$ and $\mathbb{R}^3$, and a direct method in $\mathbb{R}^3$ [Golberg, Chen and Ganesh (2000); Chen, Golberg, Ganesh and Cheng (2002)]. We discuss this method next.

As noted for splines, it suffices to find the solution to

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{d\psi_a}{dr}\right) - \lambda^2 \psi_a = \varphi(r/a) \tag{5.73}$$

and then

$$\psi_j(P) = \psi_a\left(\left\|P - P_j\right\|\right),\ 1 \le j \le N. \tag{5.74}$$

To solve (5.73), we make the change of variable

$$w = r\psi_a \tag{5.75}$$

which satisfies

$$\frac{d^2 w}{dr^2} - \lambda^2 w = r\varphi(r/a) \equiv v(r). \tag{5.76}$$

Since $p(r)$ is a piecewise polynomial, we have

$$\frac{d^2 w}{dr^2} - \lambda^2 w = r(1 - r/a)^n p(r/a),\ 0 \le r \le a, \tag{5.77}$$

and

$$\frac{d^2 w}{dr^2} - \lambda^2 w = 0,\ r > a. \tag{5.78}$$

Hence, it follows from the elementary theory of ordinary differential equations that [Derrick and Grossman (1976)]

$$w(r) = \begin{cases} Ae^{-\lambda r} + Be^{\lambda r} + q(r),\ 0 \le r \le a, \\ Ce^{-\lambda r} + De^{\lambda r},\ r > a, \end{cases} \tag{5.79}$$

where $q(r)$ is a particular solution to $w-\lambda^2 w = v(r)$ which can be chosen to be a polynomial and can be found in principle by the method of undetermined coefficients. Unfortunately, this quickly leads to very messy algebra, so we have found it advantageous to do this with symbolic ordinary differential equation (ODE) solvers, such as those in MAPLE® or MATHEMATICA®.

The four constants (A, B, C and D) in (5.79) can be chosen , so that ψ is C^2 on $[0,\infty)$. For this, it was shown in [Golberg, Chen and Ganesh (2000)] that it suffices to choose $w(0)=0$. In fact, we have the following theorem [Golberg, Chen and Ganesh (2000)].

Theorem 5.1 *Let w be a solution of* (5.78) *with* $w(0)=0$. *Then* $\psi_a = w/r$ *is twice continuously differentiable at* $r=0$ *with*

$$\psi_a(0) = w'(0),\ \psi_a'(0) = 0,$$
$$\psi_a''(0) = \frac{1}{3}\left[\lambda^2 w'(0) + p(0)\right]. \tag{5.80}$$

Furthermore, ψ_a *satisfies* (5.78) *in the sense of* $\lim r \to 0^+$.

Proof. Theorem 5.1 is proved by repeated use of l'Hospital's rule. See [Golberg, Chen and Ganesh (2000)] for details.

From Theorem 5.1 and (5.79), ψ_a is C^2 at $r=0$ if

$$A+B+q(0)=0. \tag{5.81}$$

Moreover, one can show that ψ_a is C^2 at $r=a$ if

$$\begin{cases} Ae^{-\lambda a} + Be^{\lambda a} = Ce^{-\lambda a} + De^{\lambda a}, \\ -A\lambda e^{-\lambda a} + Be^{\lambda a} + q'(a) = -C\lambda e^{-\lambda a} + D\lambda e^{\lambda a}. \end{cases} \tag{5.82}$$

Since there are four constants in (5.81)-(5.82) and three equations, one constant can be chosen arbitrarily. We choose $D=0$ and then (5.81)-(5.82) can be solved to give

$$\psi_a(r) = \begin{cases} \lambda[2B+q(0)] + q'(0), & r=0, \\ \left[Ae^{-\lambda a} + Be^{\lambda a} + q(r)\right]/r, & 0<r\le a, \\ Ce^{-\lambda a}/r, & r>a. \end{cases} \tag{5.83}$$

Note that (5.83) holds for all CS-RBFs and only $q(r)$ changes.

As examples we have the values q_1, q_2, q_3 corresponding to $\varphi_i(r)$, $i=1,2,3$ in (5.68)-(5.70) [Golberg, Chen and Ganesh (2000)].

$$q_1(r) = \frac{4}{\lambda^4\alpha} - \left(\frac{1}{\lambda^2} + \frac{6}{\lambda^4\alpha}\right) r + \frac{2}{\lambda^2\alpha} r^2 - \frac{1}{\lambda^2\alpha^2} r^3,$$

$$\begin{aligned} q_2(r) = &-\frac{480}{\alpha^3 s^6} - \frac{2880}{\alpha^5 s^8} + \left(\frac{1800}{\alpha^4 s^6} + \frac{60}{\alpha^2 s^4} - \frac{1}{s^2}\right) r \\ &- \left(\frac{240}{\alpha^3 s^4} + \frac{1440}{\alpha^5 s^6}\right) r^2 + \left(\frac{300}{\alpha^4 s^4} + \frac{10}{\alpha^2 s^2}\right) r^3 \\ &- \left(\frac{20}{\alpha^3 s^2} + \frac{120}{\alpha^5 s^4}\right) r^4 + \frac{15}{\alpha^4 s^2} r^5 - \frac{4}{\alpha^5 s^2} r^6, \end{aligned}$$

$$\begin{aligned} q_3(r) = &\frac{322560}{\lambda^8\alpha^5} + \frac{7741440}{\lambda^{10}\alpha^7} \\ &+ \left(\frac{168}{\lambda^4\alpha^2} - \frac{3}{\lambda^2} - \frac{2116800}{\lambda^8\alpha^6} \right. \\ &\left. - \frac{12700800}{\lambda^{10}\alpha^8} - \frac{25200}{\lambda^6\alpha^4}\right) r \\ &+ \left(\frac{3870720}{\lambda^8\alpha^7} + \frac{161280}{\lambda^6\alpha^5}\right) r^2 \\ &+ \left(\frac{28}{\lambda^2\alpha^2} - \frac{4200}{\lambda^4\alpha^4} - \frac{2116800}{\lambda^8\alpha^8} - \frac{352800}{\lambda^6\alpha^6}\right) r^3 \\ &+ \left(\frac{13400}{\lambda^4\alpha^5} + \frac{322560}{\lambda^6\alpha^7}\right) r^4 \\ &- \left(\frac{210}{\lambda^2\alpha^4} + \frac{17640}{\lambda^4\alpha^6} + \frac{105840}{\lambda^6\alpha^8}\right) r^5 \\ &+ \left(\frac{448}{\lambda^2\alpha^5} + \frac{10752}{\lambda^4\alpha^7}\right) r^6 - \left(\frac{2520}{\lambda^4\alpha^8} + \frac{420}{\lambda^2\alpha^6}\right) r^7 \\ &+ \frac{192}{\lambda^2\alpha^7} r^8 - \frac{35}{\lambda^2\alpha^8} r^9. \end{aligned}$$

5.6 Polynomial Particular Solutions

As we have already seen in the course of finding particular solution for $\left(\Delta - \lambda^2\right) u_p = f$ using splines, it was necessary to obtain polynomial particular solutions as well. Since polynomials are generally better understood mathematically than RBFs, it is reasonable to consider obtaining particular solutions using only polynomial approximations to f. This was first done by [Atkinson (1985)] for Poisson's equation and generalized for the Helmholtz and modified Helmholtz equations in [Golberg, Muleshkov, Chen and Cheng (2003); Muleshkov, Chen, Golberg and Cheng (2000)]. Related work can be found in [Janssen (1997)].

In general, one cannot interpolate a multidimensional polynomial on arbitrary scattered data, so a different approach is necessary than for RBF interpolation [Golberg and Chen (1996); Golberg, Muleshkov, Chen and Cheng (2003)]. In [Golberg, Muleshkov, Chen and Cheng (2003)] a standard tensor product of Chebyshev polynomials was used. To do this the physical domain is embedded in a rectangle $[a,b]\times[c,d]$ in $\mathbb{R}^2$ and in a parallelepiped $[a,b]\times[c,d]\times[e,f]$ in $\mathbb{R}^3$. Then f is approximated in $\mathbb{R}^2$ by the interpolant [Boyd (2001)]

$$f(x,y)\simeq q_{m,n}(x,y) = \sum_{i=0}^{n}\sum_{j=0}^{m} a_{ji}T_j\left(\frac{2x-b-a}{b-a}\right)T_i\left(\frac{2y-d-c}{d-c}\right) \tag{5.84}$$

where

$$a_{ji} = \frac{4}{nm\overline{c}_j\overline{c}_i}\sum_{q=0}^{n}\sum_{p=0}^{m}\frac{f(x_p,y_q)}{\overline{c}_p\overline{c}_q}\cos\left(\frac{\pi p}{n}\right)\cos\left(\frac{\pi q}{m}\right), \tag{5.85}$$

and

$$\begin{aligned} &x_p = \cos\left(\frac{p\pi}{n}\right),\ 0\le p\le n,\\ &y_q = \cos\left(\frac{q\pi}{m}\right),\ 0\le q\le m,\\ &\overline{c}_0=\overline{c}_m=2,\overline{c}_i=1,1\le i\le n-1,\\ &\overline{c}_0=\overline{c}_m=2,\overline{c}_j=1,1\le j\le m-1, \end{aligned} \tag{5.86}$$

with a similar expression $f(x,y,z)\simeq q_{n,m,p}(x,y,z)$ in $\mathbb{R}^3$. Here $T_j(x)$ and $T_i(y)$ are the Chevyshev polynomials of the first kind of degrees i,j respectively.

Then $q_{m,n}(x,y)$ and $q_{n,m,p}(x,y,z)$ are expanded in monomial form

$$q_{n,m}(x,y) = \sum_{s=0}^{n}\sum_{r=0}^{m} b_{r,s}x^r y^s \tag{5.87}$$

and

$$q_{n,m,p}(x,y,z) = \sum_{t=0}^{p}\sum_{s=0}^{n}\sum_{r=0}^{m} b_{r,s,t}x^r y^s z^t \tag{5.88}$$

and particular solutions $u_{r,s}$ and $u_{r,s,t}$ are calculated for the monomial terms $x^r y^s$ or $x^r y^s z^t$. Then particular solutions are given by

$$\hat{u}_p(x,y) = \sum_{s=0}^{n}\sum_{r=0}^{m} b_{r,s}u_{r,s} \tag{5.89}$$

and

$$\hat{u}_p(x,y,z) = \sum_{t=0}^{p}\sum_{s=0}^{n}\sum_{r=0}^{m} b_{r,s,t}u_{r,s,t} \tag{5.90}$$

The particular solutions $u_{r,s}$ and $u_{r,s,t}$ are given by the following theorems [Golberg, Muleshkov, Chen and Cheng (2003); Muleshkov, Chen, Golberg and Cheng (2000)].

Theorem 5.2 *Let* $\varepsilon\in\{-1,1\}$. *A particular solution for*

$$\Delta\psi+\varepsilon\lambda^2\psi = x^m y^n,\ m\ge 0,\ n\ge 0, \tag{5.91}$$

is given by

$$\psi(x,y) = \sum_{k=0}^{[m/2]}\sum_{l=0}^{[n/2]}\frac{\varepsilon(-\varepsilon)^{k+l}(k+l)!m!n!x^{m-2k}y^{n-2l}}{\lambda^{2k+2l+2}k!l!(m-2k)!(n-2l)!}. \tag{5.92}$$

Proof. See [Golberg, Muleshkov, Chen and Cheng (2003)].

Theorem 5.3 *A particular solution for* ($\varepsilon\in\{-1,1\}$)

$$\Delta\psi+\varepsilon\lambda^2\psi = x^p y^q z^r,\ p\ge 0,q\ge 0,r\ge 0, \tag{5.93}$$

is given by

$$\begin{aligned}&\psi(x,y,z)\\ &=\sum_{j=0}^{[p/2]}\sum_{k=0}^{[q/2]}\sum_{l=0}^{[r/2]}\\ &\frac{\varepsilon(-\varepsilon)^{k+l}(j+k+l)!p!q!r!x^{p-2j}y^{q-2k}z^{r-2l}}{\lambda^{2j+2k+2l+2}j!k!l!(p-2j)!(q-2k)!(r-2l)!}.\end{aligned} \tag{5.94}$$

Proof. See [Golberg, Muleshkov, Chen and Cheng (2003)].

In [Golberg, Muleshkov, Chen and Cheng (2003)] the monomial expressions were obtained using the symbolic code MATHEMATICA and the code for this can be found in [Golberg, Muleshkov, Chen and Cheng (2003)]. However, this led to some programming difficulties as the MATHEMATICA code had to be translated into FORTRAN for numerical purposes.

A more direct approach can be based on the fact that [Abramovitz and Stegun (1965)]

$$T_n(x) = \left(\frac{n}{2}\right) \sum_{m=0}^{[n/2]} \frac{(m-2m-1)!}{m!\,(n-2m)!} (2x)^{n-2} \tag{5.95}$$

and then the monomial expansion can be obtained by direct multiplication of these expressions. This is currently under investigation.

5.7 Trigonometric Particular Solutions

As we have already seen, using RBFs or polynomials to obtain particular solutions for the modified Helmholtz operator requires some analytic ingenuity and can lead to complex expressions if high order approximation to the source term f is required. On the other hand, if trigonometric expansions are used, then calculating the particular solution is straightforward, but obtaining rapidly convergent expansions requires some effort.

A number of authors have used this approach, but in our opinion the method of approximation has not always been mathematically correct [Reutskiy (2002)]. Hence, we follow an approach first proposed by [Atkinson (1985)] for Poisson's equation but somewhat simplified compared to his [Li and Chen (2004)].

As for polynomial approximations we embed D into a rectangle $\hat{D}$ in $\mathbb{R}^2$ or a box $\hat{D}$ in $\mathbb{R}^3$. For simplicity we assume $D = [-\pi,\pi]^d$, $d = 2,3$. We then obtain a smooth extension of f to $\hat{D}$ and then compute a rapidly convergent Fourier series approximation to $\hat{f}$.

Let $L^2\left([-\pi,\pi]^d\right)$ be the space of complex square-integrable functions on $[-\pi,\pi]^d$ and define the inner product of f and g by

$$\langle f,g\rangle = \frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} f(\mathbf{x})\,\overline{g}(\mathbf{x})\,dV. \tag{5.96}$$

To approximate $\langle f,g\rangle$ we use the quadrature rule

$$\langle f,g\rangle_n = \frac{1}{(2n)^d} \sum_{j\in Z^d(n)} f\left(\frac{\mathbf{j}\pi}{n}\right) \overline{g}\left(\frac{\mathbf{j}\pi}{n}\right) \tag{5.97}$$

for any integer $n \geq 1$ where

$$Z^d(n) = \left\{\mathbf{j} = (j_1,...,j_l) \in Z^d; -n \leq j_1,...,j_d \leq n-1\right\}. \tag{5.98}$$

Now any $f \in L^2\left([-\pi,\pi]^d\right)$ can be expanded into a Fourier series

$$f(\mathbf{x}) = \sum_{k\in Z^d} \left\langle f, e^{\mathbf{k}\cdot\mathbf{x}}\right\rangle e^{i\mathbf{k}\cdot\mathbf{x}} \tag{5.99}$$

where $\mathbf{k} = (k_1,k_2,...,k_d)$ and $\mathbf{k}\cdot\mathbf{x} = \sum_{l=1}^d x_l k_l$. Using (5.97) the Fourier expansion (5.99) can be approximated by the *hyperinterplation operator* [Sloan (1995); Golberg and Bowman (1998)]

$$L_n f(\mathbf{x}) = \sum_{\|k\|_\infty \leq n-1} \left\langle f, e^{\mathbf{k}\cdot\mathbf{x}}\right\rangle_n e^{i\mathbf{k}\cdot\mathbf{x}} \tag{5.100}$$

where $\|k\|_\infty = \max_{1\leq l\leq d} |k_l|$.

Approximation results for L_n are given in [Li and Chen (2004)]. To describe these, let

$$S_n = \text{span}\left\{e^{i\mathbf{k}\cdot\mathbf{x}}; \|k\|_\infty \leq n-1\right\}. \tag{5.101}$$

Then,

$$\|L_n f\|_2 \leq \|f\|_\infty \tag{5.102}$$

where

$$\|f\|_2 = \frac{1}{\left(\sqrt{2\pi}\right)^d} \int_{[-\pi,\pi]^d} |f|^2\,dV, \tag{5.103}$$

$$\|f\|_\infty = \sup_{\mathbf{x}\in[-\pi,\pi]^d} |f|, \tag{5.104}$$

and

$$\|f - L_n f\|_2 \leq \inf_{\chi\in S_n} \|f-\chi\|. \tag{5.105}$$

From this it follows that if f is compactly supported on $[-\pi,\pi]^d$ and f is r times continuously differentiable, then

$$\|f - L_n f\|_2 \leq c/n^r. \tag{5.106}$$

For our purposes, it suffices to use only the Fourier sine series expansion of f. Assume then that $D \subseteq [0,\pi]^d$ (This can always be done by simple translation and rescaling of variables if necessary). Let χ be a smooth function such that $\chi(\mathbf{x}) = 1$, $\mathbf{x}\in D$ and $\chi(\mathbf{x}) = 0$, $\mathbf{x}\notin [0,\pi]^d$. Let

$$f_\chi(\mathbf{x}) = f\chi(\mathbf{x}) \tag{5.107}$$

then $f_\chi = f$ for $\mathbf{x}\in D$ and f_χ is compactly supported in $[0,\pi]^d$. Extend f_χ continuously to be an odd function, i.e., $f_\chi(...,-x_l,...) = -f_\chi(...,-x_l,...)$, $1\leq l\leq d$.

Then the Fourier series of f_χ is only a sine series, i.e.,

$$f_\chi(\mathbf{x}) = \sum_{j \in Z_\pi^d} b_j(f_\chi) \sin(j_1 x_1) \cdots \sin(j_d x_d) \tag{5.108}$$

where

$$Z_\pi^d = \{\mathbf{j} = (j_1, j_2, ..., j_d) : j_1 \geq 1, ..., j_d \geq 1\} \tag{5.109}$$

and

$$b_{\mathbf{j}}(f_\chi) = \frac{1}{\pi^d} \int_{[-\pi,\pi]^d} f_\chi(\mathbf{x}) \sin(j_1 x_1) \cdots \sin(j_d x_d)\, dV. \tag{5.110}$$

Correspondingly, the hyperinterpolation operator takes the form

$$L_n(f_\chi) = \sum_{\mathbf{j} \in Z_{k-1}^d} [b_j(f_\chi)]_n \sin(j_1 x_1) \cdots \sin(j_d x_n) \tag{5.111}$$

where $Z_{n-1}^d = \{1 \leq j_1, j_2, ..., j_d \leq n-1\}$ and

$$[b_{\mathbf{j}}(f_\chi)]_n = \langle f_\chi(\mathbf{x}), \sin(j_1 x_1), \cdots, \sin(j_d x_d) \rangle_n \tag{5.112}$$

Using $L_n(f_\chi)$ to approximate the source term f, it can be verified by direct differentiation that the corresponding particular solutions are given by

$$\hat{u}_p(x,y) = -\sum_{1 \leq j_1, j_2 \leq n-1} \frac{[b_j(f_\chi)]_n}{j_1^2 + j_2^2 + \lambda^2} \sin(j_1 x) \sin(j_2 y), \text{ in } \mathbb{R}^2 \tag{5.113}$$

and

$$\hat{u}_p(x,y,z) = -\sum_{1 \leq j_1, j_2, j_3 \leq n-1} \frac{[b_j(f_\chi)]_n}{j_1^2 + j_2^2 + j_3^2 + \lambda^2} \sin(j_1 x) \sin(j_2 y) \sin(j_3 z), \text{ in } \mathbb{R}^3. \tag{5.114}$$

Last, we point out that the hyperinterpolation operator $L_n(f_\chi)$ can be calculated efficiently by using the fast Fourier transform. Details can be found in [Li and Chen (2004)].

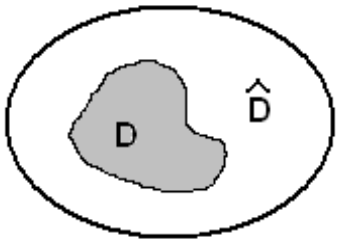

Figure 6.1: D and bounded domain $\hat{D}$

6 Trefftz Bases

Having discussed how to obtain particular solutions, we now turn to the issue of determining appropriate Trefftz bases for solving the homogeneous boundary value problem.

Generally, Trefftz bases fall into two broad classes, F-Trefftz bases based on fundamental solutions for $\Delta - \lambda^2$ and T-Trefftz bases, which are usually obtained by separation of variables. T-Trefftz bases can also be generated by the application of Bergman-Vekua operators [Bergman and Shiffer (1953); Bergman and Herriot (1965); Vekua (1967); Melenk (1995); Melenk and Babuška (1995)] which are discussed in Section 6.5. This latter approach is interesting because it can be used to generate bases for operators with non-constant coefficients [Bergman and Shiffer (1953); Bergman and Herriot (1965); Vekua (1967); Melenk (1995); Melenk and Babuška (1995)].

6.1 The Method of Fundamental Solutions

In our work we have focussed on F-Trefftz bases giving rise to what is usually called the *method of fundamental solutions* (MFS) [Golberg and Chen (1996, 1998); Limic (1981); Alves (2000)]. This method may be viewed as a version of the boundary integral equation method as shown in [Golberg and Chen (1998)]. This technique was pioneered by [Kupradze and Aleksidze (1964)] and was, until recently, limited to solving homogeneous elliptic problems.

To begin a description of the method, we assume that D is bounded, connected and simply connected. Let $\hat{D}$ be a bounded domain containing D as shown in Figure 6.1.

Let $\hat{S}$ be the boundary of $\hat{D}$ and let $\{Q_j\}_{j=1}^N$ be N distinct

points on $\hat{S}$ and define

$$v_N(p) = \sum_{j=1}^{N} a_j G(P,Q_j;\lambda),\ P \in D \cup S \tag{6.1}$$

where $G(P,Q_j,\lambda)$ is a fundamental solution of $\Delta - \lambda^2$. Since $\left(\Delta-\lambda^2\right) G(P,Q_j;\lambda) = 0,\ P \neq Q$, then $\left(\Delta-\lambda^2\right) v_N = 0,\ P \in D \cup S$. In [Alves (2000)] it was shown that if $\left\{Q_j\right\}_{j=1}^{\infty}$ is dense in $\hat{S}$, then the set $\left\{G(P,Q_j;\lambda)\right\}_{j=1}^{\infty}$ is complete in the set $X = \left\{\left(\Delta-\lambda^2\right) v = 0\right\}$. Hence, $\left\{G(P,Q_j;\lambda)\right\}_{j=1}^{\infty}$ is a Trefftz basis for X.

As noted in Section 4, the coefficients $\left\{a_j\right\}_{j=1}^{N}$ in (6.1) can be chosen by collocation, least squares or Galerkin's method. In our work we have generally used collocation, although other methods are also being investigated.

As shown in Section 4, for collocation we choose N points on S and set

$$Bv_N(P_k) = g(P_k) - Bu_p(P_k),\ 1 \le k \le N. \tag{6.2}$$

Using (6.1) in (6.2) gives the N linear equations

$$\sum_{j=1}^{N} a_j BG(P_k,Q_j;\lambda) = g(P_k) - Bu_p(P_k),\ 1 \le k \le N. \tag{6.3}$$

These equations can then be solved by direct solvers such as Gaussian elimination. However, this requires care, since the matrix

$$\mathbf{A}_c = [BG(P_k,Q_j)],\ 1 \le j,k \le N, \tag{6.4}$$

can be highly ill-conditioned [Schaback (1995); Kitagawa (1988, 1991); Ramachandran (2002)]. Generally, the condition number of $\mathbf{A}_c$ increases as the distance of $\hat{S}$ from S increases. At the same time the accuracy of the MFS increases under these same circumstances. At present, the optimal location of the source points is not known but generally we have found that choosing the distance of $\hat{S}$ from S at most three times the diameter of D seems to give good results [Golberg and Chen (1998)]. Moreover, it usually is satisfactory to choose the source points uniformly distributed on a circle of radius R in $\mathbb{R}^2$ and uniformly on a sphere of radius R in $\mathbb{R}^3$ [Golberg and Chen (1998); Bogomolny (1985); Katsurada and Okamoto (1996)].

Because there is some uncertainty about the effect of the ill-conditioning of $\mathbf{A}_c$, we have begun investigating methods to mitigate this problem. These are based on ideas drawn from statistical analysis.

Many of these methods are based on the singular value decomposition (SVD) of $\mathbf{A}_c$. This approach was first examined by [Kitagawa (1988, 1991)] for Laplace's equation and more recently by [Ramachandran (2002)]. Here we extend these ideas to the modified Helmholtz equation.

As is well-known an $N \times N$ matrix $\mathbf{A}$ can be decomposed as [Golberg and Cho (2004)]

$$\mathbf{A} = \mathbf{U}\mathbf{D}\mathbf{V}^T \tag{6.5}$$

where $\mathbf{U}$ and $\mathbf{V}$ are orthogonal matrices and $\mathbf{D}$ is the diagonal matrix of singular values of $\mathbf{A}$. Let $\mu_i, 1 \le i \le N$ be the singular values assumed to be ordered in decreasing order; i.e., $\mu_1 \ge \mu_2 \ge \cdots \ge \mu_N$ and μ_i are the eigenvalues of $\mathbf{A}^T\mathbf{A}$.

Using (6.5), the solution of $\mathbf{A}\mathbf{x} = \mathbf{y}$ can be obtained as follows. Since the columns of $\mathbf{V}$ span $\mathbb{R}^N$,

$$\mathbf{x} = \sum_{i=1}^{N} a_i \mathbf{v}_i \tag{6.6}$$

where $\{\mathbf{v}_i\}_{i=1}^{N}$ are the columns of $\mathbf{V}$. From (6.5) $\mathbf{A}\mathbf{v}_i = \mu_i \mathbf{u}_i$ where $\mathbf{u}_i$ are the columns of $\mathbf{U}$. Then,

$$\mathbf{y} = \mathbf{A}\mathbf{x} = \sum_{i=1}^{N} a_i \mathbf{A}\mathbf{v}_i = \sum_{i=1}^{N} a_i \mu_i \mathbf{u}_i. \tag{6.7}$$

Since $\{\mathbf{u}_i\}_{i=1}^{N}$ are orthogonal,

$$a_i = \langle \mathbf{y}, \mathbf{u}_i \rangle / \mu_i\ 1 \le i \le N, \tag{6.8}$$

which gives

$$\mathbf{x} = \sum_{i=1}^{N} \frac{\langle \mathbf{y}, \mathbf{u}_i \rangle \mathbf{v}_i}{\mu_i} \tag{6.9}$$

as the SVD of the solution $\mathbf{x}$.

This expression can be used to analyze the propagation of error in the solution of $\mathbf{A}\mathbf{x} = \mathbf{y}$. Suppose $\mathbf{y}$ is perturbed by a vector $\Delta\mathbf{y}$, i.e., $\mathbf{y} \to \mathbf{y} + \Delta\mathbf{y}$, then the solution $\mathbf{x}$ is perturbed by

$$\Delta\mathbf{x} = \sum_{i=1}^{N} \frac{\langle \Delta\mathbf{y}, \mathbf{u}_i \rangle \mathbf{v}_i}{\mu_i} \tag{6.10}$$

so that

$$\|\Delta \mathbf{x}\| \leq \sum_{i=1}^{N} \frac{|\langle \Delta \mathbf{y}, \mathbf{u}_i \rangle|}{\mu_i} \|\mathbf{v}_i\| \leq \sum_{i=1}^{N} \frac{\|\Delta \mathbf{y}\| \|\mathbf{u}_i\| \|\mathbf{v}_i\|}{\mu_i}. \quad (6.11)$$

Since $\|\mathbf{u}_i\| = \|\mathbf{v}_i\| = 1, 1 \leq i \leq N$, $\|\Delta \mathbf{x}\| \leq \sum_{i=1}^{N} \|\Delta \mathbf{y}\| / \mu_i$. Hence, the error $\|\Delta \mathbf{y}\|$ is magnified by $1/\mu_i$, $1 \leq i \leq N$. Since ill-conditioning is indicated by small singular values, error propagation can be reduced by dropping the terms in (6.11) satisfying $\mu_i \leq \varepsilon$, where $\varepsilon (> 0)$ is some pre-assigned error value. Hence, to reduce the effect of ill-conditioning we approximate $\mathbf{x}$ by

$$\hat{\mathbf{x}} = \sum_{i=1}^{M} \frac{\langle \mathbf{y}, \mathbf{u}_i \rangle \mathbf{v}_i}{\mu_i} \quad (6.12)$$

where $\mu_i \leq \varepsilon$ for $i > M$. $\hat{\mathbf{x}}$ is called the *truncated singular value decomposition* (TSVD) of $\mathbf{x}$. Of course, this increases the truncation error.

$$\mathbf{x} - \hat{\mathbf{x}} = \sum_{i=M+1}^{N} \frac{\langle \mathbf{y}, \mathbf{u}_i \rangle \mathbf{v}_i}{\mu_i}. \quad (6.13)$$

The expectation is that if the values $\langle \mathbf{y}, \mathbf{u}_i \rangle$ are small, the truncation error will be small while the propagation of round-off error is mitigated by using $\hat{\mathbf{x}}$ instead of $\mathbf{x}$.

As has been observed experimentally, the MFS has the somewhat surprising property that the ill-conditioning often seems to have little effect on the numerical accuracy of $\mathbf{x}$. As yet, there seems to be no general rigorous explanation of this fact. An heuristic explanation of this fact follows.

First, note that the solution of (6.13) is not of primary importance, rather the approximate solution of the boundary value problem is. Letting

$$\mathbf{c} = [G(P, Q_1), G(P, Q_2), ..., G(P, Q_N)]^T, \; P \in D \cup S, \quad (6.14)$$

$$v_N(P) = \langle \mathbf{c}, \mathbf{x} \rangle, \; P \in D \cup S. \quad (6.15)$$

Using the SVD of $\mathbf{x}$

$$v_N(P) = \sum_{i=1}^{N} \frac{\langle \mathbf{y}, \mathbf{u}_i \rangle \langle \mathbf{c}, \mathbf{v}_i \rangle}{\mu_i}. \quad (6.16)$$

Assume now that $\mu_i, i \geq M+1$ are the small singular values of $\mathbf{A}$ and $\langle \mathbf{c}, \mathbf{v}_i \rangle = 0, i \geq M+1$. Then

$$v_N(P) = \sum_{i=1}^{M} \frac{\langle \mathbf{y}, \mathbf{u}_i \rangle \langle \mathbf{c}, \mathbf{v}_i \rangle}{\mu_i}. \quad (6.17)$$

Hence, the effect of small singular values has been eliminated. Since we do not expect this to hold exactly, it suggests an alternative procedure to mitigate the effect of the small singular values.

Write

$$v_N(P) = \sum_{i=1}^{N} \frac{\langle \mathbf{y}, \mathbf{u}_i \rangle}{\mu_i / \langle \mathbf{c}, \mathbf{v}_i \rangle} \equiv \sum_{i=1}^{N} \frac{\langle \mathbf{y}, \mathbf{u}_i \rangle}{\sigma_i}, \; P \in D \cup S. \quad (6.18)$$

Now order $|\sigma_i|, 1 \leq i \leq N$ in decreasing order and for simplicity assume that $|\sigma_1| \geq |\sigma_2| \geq \cdots \geq |\sigma_N|$. If M is chosen such that $|\sigma_i| < \varepsilon, i > M$, then v_N is approximated by

$$\hat{v}_N(P) = \sum_{i=1}^{M} \frac{\langle \mathbf{y}, \mathbf{u}_i \rangle}{\sigma_i}, \; P \in D \cup S. \quad (6.19)$$

We now expect $\hat{v}_N(P)$ to be more computationally stable than $v_N(P)$.

Other approaches to mitigating the ill-conditioning can be based on least squares and Galerkin methods. Before discussing this, we first examine the cause of the ill-conditioning of $\mathbf{A}$. Let

$$\mathbf{r}_j = (BG(P_j, Q_1), G(P_j, Q_2), ..., G(P_j, Q_N)) \quad (6.20)$$

be the j-th row of $\mathbf{A}$. Since G is a function of the Euclidean distance $\|P - Q\|$ between P and Q, $\mathbf{r}_j$ depends on the distances $\|P_j - Q_k\|, 1 \leq k \leq N$, as shown in Fig. 6.2. Also the $(j+1)$-th row is

$$\mathbf{r}_{j+1} = (BG(P_{j+1}, Q_1), G(P_{j+1}, Q_2), ..., G(P_{j+1}, Q_N)) \quad (6.21)$$

which depends on the distances $\|P_{j+1} - Q_k\|, 1 \leq k \leq N$. Now as R increases, the distance $\|P_j - Q_k\|, 1 \leq k \leq N$ and $\|P_{j+1} - Q_k\|, 1 \leq k \leq N$ become approximately equal. Hence, adjacent rows of $\mathbf{A}$ become approximately equal and $\mathbf{A}$ becomes increasingly ill-conditioned. A similar argument holds as N increases and adjacent source points become closer together. Thus, a possible strategy for reducing ill-conditioning is to try to satisfy the boundary conditions as well as possible using a small number of source points. This suggests choosing a larger number of field points $\{P_j\}_{j=1}^{M}$ than source points $\{Q_j\}_{j=1}^{M}$ and satisfying the boundary conditions, in a least squares sense as indicated in Section 4.1. In this case, we approximate v by

$$v_N(P) = \sum_{k=1}^{N} a_k G(P, Q_k; \lambda) \quad (6.22)$$

where $\{a_k\}_{k=1}^N$ are obtained by solving

$$\mathbf{A}_L^T\mathbf{A}_L\mathbf{a} = \mathbf{A}_L^T\mathbf{y} \tag{6.23}$$

where

$$\mathbf{A}_L = [BG(P_j, Q_k; \lambda)],\ 1 \le j \le M, 1 \le k \le N \tag{6.24}$$

where $M \ge N$ and

$$\mathbf{y} = [g(P_j) - Bu_p(P_j)],\ 1 \le j \le M. \tag{6.25}$$

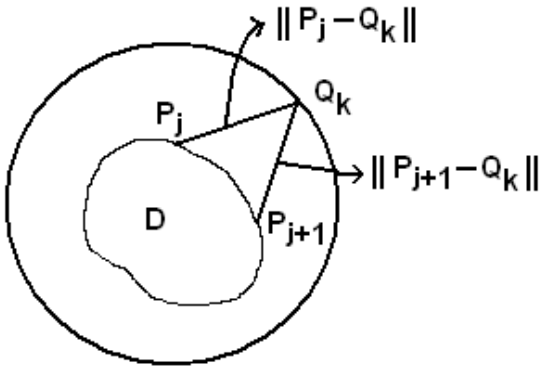

Figure 6.2: Source to field point distances

Unfortunately, $\mathbf{A}_L^T\mathbf{A}_L$ can still be badly ill-conditioned. Again, the ill-conditioning can be mitigated by using various techniques from statistical analysis. These, as before, can be based on the SVD of $\mathbf{A}_L^T\mathbf{A}_L$. In this case,

$$\mathbf{A}_L^T\mathbf{A}_L = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^T \tag{6.26}$$

where $\mathbf{U}$ is orthogonal and $\mathbf{\Lambda}$ is a diagonal matrix whose diagonal elements are the eigenvalues of $\mathbf{A}_L^T\mathbf{A}_L$. Typical methods are based on *Tikhonov regularization* [Tikohnov and Arsenin (1977)] which is also known as *ridge regression* [Golberg and Cho (2004)] in the statistical literature. Here we consider determining the *regularized solution* $\mathbf{x}_R$ by solving

$$\mathbf{x}_R = \arg\min \|\mathbf{A}_L\mathbf{x} - \mathbf{y}\|^2 + k\|\mathbf{x}\|^2,\ k > 0, \tag{6.27}$$

where $k > 0$ is a *regularization parameter*.

In this case, $\mathbf{x}_R$ satisfies

$$\left(\mathbf{A}_L^T\mathbf{A}_L + k\mathbf{I}\right)\mathbf{x}_R = \mathbf{A}_L^T\mathbf{y}. \tag{6.28}$$

For $k = 0$, $\mathbf{x}_R$ satisfies (6.23). In general, for $k > 0$, $\mathbf{A}_L^T\mathbf{A}_L + k\mathbf{I}$ is better conditioned than $\mathbf{A}_L^T\mathbf{A}_L$. However, as k increases, the error $\|\mathbf{x} - \mathbf{x}_k\|$ increases as well. Using statistical ideas it is possible to calculate the optimal value of k [Golberg and Cho (2004)]. Two of the most popular techniques are *generalized cross validation* (GCV) [Wahba (1990)] and Hansen's L-curve [Hansen (1992)]. Again, both of these procedures are based on the SVD of $\mathbf{A}_L^T\mathbf{A}_L$, which is just the usual spectral decomposition of a symmetric matrix $\mathbf{A}_L^T\mathbf{A}_L$.

Hence,

$$\mathbf{x}_R = \sum_{i=1}^{N} \frac{\langle \mathbf{A}_L^T\mathbf{y}, \mathbf{u}_i \rangle}{\mu_i^2 + k} \tag{6.29}$$

where $\{\mu_k^2\}_{k=1}^N$ are the singular values of $\mathbf{A}_L^T\mathbf{A}_L$ and $\mathbf{u}_i, 1 \le i \le N$ are the columns of $\mathbf{U}$. Details of the GCV can be found in [Wahba, Golub and Health (1979); Wahba (1990)].

In the L-curve one plots the points

$$\left(\log\|\mathbf{x}_R\|^2,\ \log\|\mathbf{A}_L\mathbf{x}_R - \mathbf{y}\|^2\right) \tag{6.30}$$

and the resulting curve has the L shape shown in Figure 6.3.

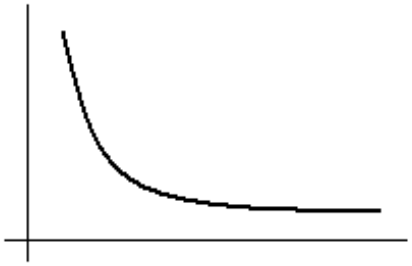

Figure 6.3: L-curve

The optimum value of k corresponds to the "knee" of the curve. Note that this plot can be obtained efficiently using (6.29), since it requires only the one time computation of the SVD of $\mathbf{A}_L$.

An alternative least squares procedure is to assume that the source points $\{Q_j\}_{k=1}^N$ are not fixed but are chosen simultaneously with the source strengths $\{a_k\}_{k=1}^N$ in (6.1) [Fairweather and Karageorghis (1998)]. In this case, $\|\mathbf{A}_L\mathbf{x} - \mathbf{y}\|^2$ is minimized with respect to $\left(\{a_k\}_{k=1}^N, \{Q_k\}_{k=1}^N\right)$. This method is computationally more intensive than either collocation or least squares with fixed sources, particularly in $\mathbb{R}^3$. Hence, we would generally not recommend it for use in time dependent problems.

6.2 Galerkin's Method

As we pointed out in Section 4, the boundary conditions can be satisfied using the inner product given in (4.24). We expect this method to be more stable than collocation, particularly if the basis is orthonormal as indicated in [Bergman and Herriot (1961)].

6.3 Multiply Connected and Unbounded Domains

If D is a bounded, multiply connected domain as shown in Fig. 6.4, then sources need to be placed in the interior of the holes in D as well in the unbounded component of the complement of D in order to satisfy the boundary conditions. In general, the interior sources should be placed far from the interior boundaries. At present, we are unaware of any theory which determines how to distribute the sources between the interior and the exterior domains. However, it has been found experimentally that it is best to put most of the sources in the exterior domain. As for simply connected domains, the boundary conditions can be satisfied using either collocation, least squares or Galerkin's method.

If D is simply connected and unbounded, then sources should be placed in the bounded complement of D with increasing accuracy usually being obtained the further the sources are from the boundary S.

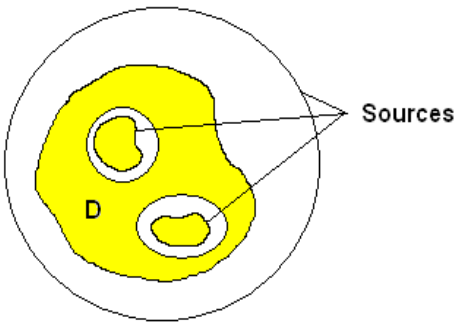

Figure 6.4: Source points for a multiply connected domain

6.4 Singular Solutions

So far we have assumed that the solution to the boundary value problem is smooth. However, if either the boundary S or the boundary data g is not smooth, the solution to that boundary value problem can develop singularities in the neighborhood of the singular points. Since the fundamental solution $G(P,Q;\lambda)$ is C^∞ for $P \neq Q$, the approximate solution v_N in (6.1) is C^∞ as well and we will not obtain a good approximation to solutions which are not C^∞. This same problem occurs in the BEM and in domain based methods such as the FEM [Strang and Fix (1973); Fix, Gulati and Wakoff (1973)]. How to deal with this problem is not totally resolved. In [Karageorghis (1992)], this problem was addressed for Laplace's equation in 2D and [Tolley (1977)] and [Discroll (1995)] considered this issue for the ordinary Helmholtz equation. The basic idea is to determine the asymptotic behavior of the solution near the singular points and then add functions to the MFS expansion which display this singular behavior. For example, if D is a polygon and $P \in S$ is a vertex with interior angle α/π, then the functions $I_{n\alpha}(\lambda r)\cos(n\alpha\theta)$, $I_{n\alpha}(\lambda r)\sin(n\alpha\theta)$ are solutions to $(\Delta - \lambda^2)v = 0$, where (r,θ) is a polar coordinate system centered at P. Then, in a neighborhood of P, we can approximate v by an expression of the form

$$
\begin{aligned}
&v_N(P) \\
&= \sum_{k=1}^{N} a_k G(P,Q_k;\lambda) + \sum_{n=0}^{M} b_n I_{n\alpha}(\lambda r)\cos(n\alpha\theta) \\
&\quad + \sum_{n=1}^{M} c_n I_{n\alpha}(\lambda r)\sin(n\alpha\theta). \qquad (6.31)
\end{aligned}
$$

To solve the global problem the domain can be decomposed in such a way that only one vertex occurs in each subdomain as shown in Figure 6.5. Then, we introduce an expansion of the form (6.31) in each subdomain D_i. Boundary conditions can be satisfied by collocation and by requiring continuity of v and the normal derivative of v across the element interfaces.

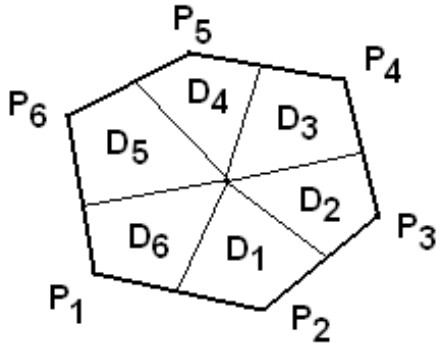

Figure 6.5: Decomposition of D and subdomains

For problems in $\mathbb{R}^3$, simple analytic expressions for the singular functions do not seem to be available so this approach does not appear to be feasible [Grisvard (1992)]. At present, in analogy with the BEM, mesh grading of collocation points may be possible as has been done for some $2D$ problems in [Karageorghis and Fairweather (1987)]. As yet, no results seems to have been published using such an approach.

6.5 T-Trefftz Bases

6.5.1 Bases in $\mathbb{R}^2$

We begin by assuming that D is a bounded, connected and simply connected domain in $\mathbb{R}^2$ and assume that the solution to the boundary value problem

$$\begin{cases} \Delta v - \lambda^2 v = 0 \\ Bv = g - Bu_p \end{cases} \tag{6.32}$$

is smooth. Assume in addition that the origin of coordinates is located at the centroid of D. Introduce polar coordinates (r,θ) with $r=0$ at the centroid of D. Then it is known that the set

$$\{I_n(\lambda r)\cos n\theta\}_{n=0}^{\infty} \cup \{I_n(\lambda r)\sin n\theta\}_{n=1}^{\infty}, \tag{6.33}$$

where I_n is the Bessel function of second kind and order n, is complete in the set of solutions of $\Delta v - \lambda^2 v = 0$ [Melenk (1995); Melenk and Babuška (1995)]. Hence, to approximate the solution to (6.32)-(6.33) we define

$$v_N = \sum_{n=0}^{N} a_n I_n(\lambda r)\cos n\theta + \sum_{n=1}^{N} b_n I_n(\lambda r)\sin n\theta. \tag{6.34}$$

By definition, $\Delta v_N - \lambda^2 v_N = 0$, so we need to pick the constants $\{a_k\}_{k=0}^{N}$ and $\{b_k\}_{k=1}^{N}$ to satisfy the boundary conditions in (6.32). As for the MFS, this can be done by using either collocation, least squares or Galerkin's method. As before, this leads one to solve a system of $2N+1$ linear equations. These equations are generally ill-conditioned, so that methods based on the SVD should be preferable to straightforward Gaussian elimination.

In contrast to the MFS, it is possible to obtain good estimates of the approximation orders of the T-Trefftz bases (6.34). This can be done by using the Bergman-Vekua theory of integral operator [Bergman and Shiffer (1953); Bergman and Herriot (1961, 1965); Melenk (1995); Melenk and Babuška (1995)].

The basic idea is that given a complete set of solutions of Laplace's equation $\Delta u = 0$ these can be mapped onto a complete set of solutions to $\Delta v - \lambda^2 v = 0$. In particular, if $u_0(x,y)$ is a complex holomorphic solution to $\Delta v = 0$, then

$$V(x,y) = u_0(x,y) - \int_0^1 u_0(tx,ty)\frac{\partial}{\partial t} I_0\left(\lambda r\sqrt{1-t}\right) dt \tag{6.35}$$

is a solution of $\Delta v - \lambda^2 v = 0$ [Bergman and Herriot (1961, 1965); Melenk (1995); Melenk and Babuška (1995)].

If we consider

$$u_0(x,y) \in S = \left\{1, z, \overline{z}, z^2, \overline{z^2}, ..., z^n, \overline{z^n}, ...\right\} \tag{6.36}$$

where $z = x+iy$ and $\overline{z} = x-iy$, then S is a complete set of holomorphic solutions to $\Delta u = 0$.Then, it can be shown that

$$V(z^n) = c_n(\lambda) e^{in\theta} I_n(\lambda r) \tag{6.37}$$

and

$$V(\overline{z}^n) = c_n(\lambda) e^{-in\theta} I_n(\lambda r) \tag{6.38}$$

where $\{c_n(\lambda)\}$ are appropriate constants, is a complete set of complex solutions of $\Delta v - \lambda^2 v = 0$, where $z = re^{i\theta}$. Then,

$$I_n(\lambda r)\cos n\theta = \frac{V(z^n) + V(\overline{z}^n)}{2c_n(\lambda)} \tag{6.39}$$

and

$$I_n(\lambda r)\sin n\theta = \frac{V(z^n) - V(\overline{z}^n)}{2c_n(\lambda)} \tag{6.40}$$

is a complete set of real solutions to $\Delta v - \lambda^2 v = 0$.

Using classical error estimates for approximation by harmonic polynomials, i.e., elements in span S, and the fact that (6.35) is a bounded operator in appropriate Banach spaces of functions, enables one to obtain error estimates for approximation by the Trefftz basis (6.33). A classical result of this type is given below.

Theorem 6.1 [Mergelyan (1962)] *Let $D \subseteq \mathbb{R}^2$ be a simply connected, bounded Liponitz domain with boundary S. Let $\hat{D}$ be such that $D \cup S \subseteq \hat{D}$ and assume that*

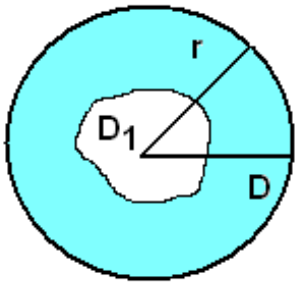

Figure 6.6: D with a single hole

$f \in L^2\left(\hat{D}\right)$ is holomorphic in $\hat{D}$. Then, there exists a harmonic polynomial φ_p of degree p such that

$$\|f-\varphi_p\|_\infty \le c_1 e^{-\gamma p}\|f\|_2, \tag{6.41}$$

and

$$\left\|f'-\varphi_p'\right\|_\infty \le c_2 e^{-\gamma p}\|f\|_2,\ \gamma>0, \tag{6.42}$$

where c_1 and c_2 do not depend on φ_p.

Using Theorem 6.1 and the boundedness of (6.38) in L^∞, it follows that if v is a holomorphic solution of $\Delta v-\lambda^2 v=0$, there exists a function of the form (6.34) such that

$$\|v-v_N\|_\infty \le c_1 e^{-\gamma N}\|f\|_2, \tag{6.43}$$

and

$$\left\|v'-v_N'\right\|_\infty \le c_2 e^{-\gamma N}\|f\|_2, \gamma>0. \tag{6.44}$$

In [Melenk (1995)] and [Melenk and Babuška (1995)], more general theorems with relaxed smoothness conditions on v are given. We refer the reader there for details.

Using these results, one can obtain error estimates for the Trefftz approximation v_N to v provided that the coefficients $\{a_k\}_{k=0}^N \cup \{b_k\}_{k=1}^N$ are chosen by using Galerkin's method.

If D is multiply connected, then using T-Trefftz bases becomes increasingly complex. For example, suppose D is bounded with a single hole as shown in Figure 6.6 and assume that we have a polar coordinate system with the origin at the centroid of D_1.

Then, the corresponding Trefftz basis will contain terms of the form

$$\{K_n(\lambda r)\cos n\theta\}_{n=0}^{N_1} \cup \{K_n(\lambda r)\sin n\theta\}_{n=1}^{N_1} \tag{6.45}$$

where by letting $\lambda r = z$,

$$\begin{aligned} &K_n(z) \\ &= \frac{1}{2}\left(\frac{1}{2}z\right)^{-n}\sum_{k=0}^{n-1}\frac{(n-k-1)!}{k!}\left(-\frac{1}{4}z^2\right)^k \\ &+(-1)^{n+1}\ln\left(\frac{1}{2}z\right)I_n(z) \\ &+(-1)^n\frac{1}{2}\left(\frac{1}{2}z\right)^n \\ &\sum_{k=0}^{\infty}\left[\psi(k+1)+\psi(n+k+1)\right]\frac{\left(\frac{1}{4}z^2\right)^k}{k!\,(n+k)!} \end{aligned} \tag{6.46}$$

are Bessel functions of the third kind [Abramovitz and Stegun (1965)], where $\psi(z)=\Gamma'(z)/\Gamma(z)$ is called the digamma function; $\psi(1)=-\gamma$ and $\psi(n)=-\gamma+\sum_{k=1}^{n-1}k^{-1}$ for $n\ge 2$ (γ is Euler's constant).

Generally, for each hole one needs to add corresponding terms of the form (6.45) to the Trefftz expansion centered at the centroids of each hole. In this regard, using T-Trefftz bases appears to be more difficult than the MFS.

As for the MFS, care needs to be taken if the solution has singularities either due to geometric singularities or singularities due to the boundary data g. As there, the best approach is to determine the asymptotic behavior of the solution in the neighborhood of the singular points and add singular functions to the Trefftz expansion as for the MFS.

Although we have approached T-Trefftz basis for $\Delta-\lambda^2$ by Bergman-Vekua operators, the more classical approach is to observe that the basis (6.33) can be obtained by separation of variables of $\Delta v-\lambda^2 v=0$ in polar coordinates. This suggests that other Trefftz bases can be obtained by separation of variables in other coordinate systems. In particular, if Cartesian coordinates are used, one can look for solutions in the form

$$v(x,y)=A\exp(\alpha x+\beta y). \tag{6.47}$$

Substituting (6.47) into $\Delta v-\lambda^2 v=0$ gives $\alpha^2+\beta^2-\lambda^2=0$, so $\alpha^2+\beta^2=\lambda^2$. Hence, (α,β) must lie on a circle with radius λ. If we choose

$$(\alpha_{N,k},\beta_{N,k})=\lambda\left(\cos\frac{2\pi k}{N},\sin\frac{2\pi k}{N}\right),\ 0\le k\le N-1, \tag{6.48}$$

then we conjecture that the set

$$\bigcup_{N=1}^{\infty}\bigcup_{k=0}^{N-1}(\alpha_{N,k},\beta_{N,k}) \tag{6.49}$$

is a Trefftz basis for $\Delta v-\lambda^2 v=0$. This result is known to be true for the ordinary Helmholtz equation $\Delta v+\lambda^2 v=0$ where λ in (6.48) is replaced by $i\lambda$, $i^2=-1$ [Melenk (1995); Melenk and Babuška (1995)]. We expect this basis to be more efficient than the standard T-Trefftz and MFS bases, since it does not require the calculation of Bessel functions.

6.5.2 *Bases in* $\mathbb{R}^3$

For simplicity, we restrict our discussion to the case where D is a bounded, connected and simply connected domain in $\mathbb{R}^3$ and assume that the solution to the boundary value problem (4.4)-(4.5) is smooth.

Letting (r,θ,φ) be spherical polar coordinates in $\mathbb{R}^3$, then it is known that the functions

$$\begin{aligned}&\{i_m(\lambda r)P_m^n(\cos\theta)\sin(n\varphi)\,,\\ &i_m(\lambda r)P_m^n(\cos\theta)\cos(n\varphi)\},\\ &-m\le n\le m, m=0,1,2,..\end{aligned} \tag{6.50}$$

is a Trefftz basis for solutions of $\Delta v-\lambda^2 v=0$. Here, $i_m(\lambda r)$ is the spherical Bessel function of the second kind of order u and $P_m^n(\cos\theta)$ are the associated Legendre functions [Golberg and Chen (1996); Cheung, Jin and Zienkiewicz (1991)]. Thus, we can obtain approximate solutions of the form

$$\begin{aligned}v_N(P)=&\sum_{m=0}^{N}\sum_{n=-m}^{m}a_{m,n}i_m(\lambda r)P_m^n(\cos\theta)\sin(n\varphi)\\ &+\sum_{m=0}^{N}\sum_{n=-m}^{m}b_{m,n}i_m(\lambda r)P_m^n(\cos\theta)\cos(n\varphi)\,.\end{aligned} \tag{6.51}$$

As in $\mathbb{R}^2$, the constants $\{a_{m,n}\}$ and $\{b_{m,n}\}$ are obtained by satisfying the boundary conditions either by collocation, least squares or Galerkin's method.

As in $\mathbb{R}^2$, there is a generalization of the Bergman-Vekua theory which enables one to obtain the bases (6.50) as the image of harmonic polynomials under an appropriate integral operator. Details can be found in [Tjong (1970); Colton (1971); Gilbert and Lo (1971)]. The completeness of (6.50) can be established using this fact. However, sharp error bounds do not seem to be available as in $\mathbb{R}^2$.

As in $\mathbb{R}^2$, we can consider obtaining alternative bases by separating variables in Cartesian rather than polar coordinates. Hence, we look for solutions to $\Delta v-\lambda^2 v=0$ in the form

$$v=A\exp(\alpha x+\beta y+\gamma z)\,. \tag{6.52}$$

Substituting (6.52) into $\Delta v-\lambda^2 v=0$ we find that (α,β,γ) satisfy

$$\alpha^2+\beta^2+\gamma^2=\lambda^2 \tag{6.53}$$

so that (α,β,γ) lies on a sphere of radius λ in $\mathbb{R}^3$. As in $\mathbb{R}^2$, we conjecture that if $\{(\alpha_k,\beta_k,\gamma_k)\}_{k=1}^{\infty}$ is a dense subset of this sphere, then the set

$$\{\exp(\alpha_k x+\beta_k y+\gamma_k z)\}_{k=1}^{\infty} \tag{6.54}$$

is a Trefftz basis for $\Delta v-\lambda^2 v=0$. This suggests choosing

$$\alpha_{j,k}=\lambda\sin\frac{\pi j}{n}\cos\frac{2\pi k}{m},\ 0\le j\le n-1,\ 0\le k\le m-1 \tag{6.55}$$

$$\beta_{j,k}=\lambda\sin\frac{\pi j}{n}\sin\frac{2\pi k}{m},\ 0\le j\le n-1,\ 0\le k\le m-1 \tag{6.56}$$

$$\gamma_j=\lambda\sin\frac{\pi j}{n},\ 0\le j\le n-1,\ (n,m)\ge 1 \tag{6.57}$$

as appropriate points on the sphere of radius λ to use in (6.54). This basis should be computationally more efficient than the classical basis (6.50), since it does not require the calculation of special functions.

7 Numerical Results

In this section, we present several numerical examples illustrating our methodology. For simplicity, we restrict ourselves to the RBF spline-MFS for the diffusion equation.

Example 7.1 Consider the following parabolic equation

$$\frac{\partial u}{\partial t}=\Delta u+f(x,y,t) \tag{7.1}$$

in the domain $[0,1]\times[0,1]$. The forcing term is given by

$$f(x,y,t)=\sin x\sin y(2\sin t+\cos t). \tag{7.2}$$

The initial and boundary conditions correspond to the solution

$$u(x,y,t) = \sin x \sin y \sin t. \tag{7.3}$$

This example was considered by Ingber and Phan-Thien [Ingber and Phan-Thien (1992)] using a boundary element method. To approximate the forcing term f, we chose 48 interpolation points (see Figure 7.1) in which 32 boundary points were used as the collocation points for the MFS. We chose polyharmonic splines of order two $(r^4 \log r)$ as the basis function. To evaluate the homogeneous solution using the MFS, we chose 32 source points on a circle with center at $(0.5, 0.5)$ and radius 2.

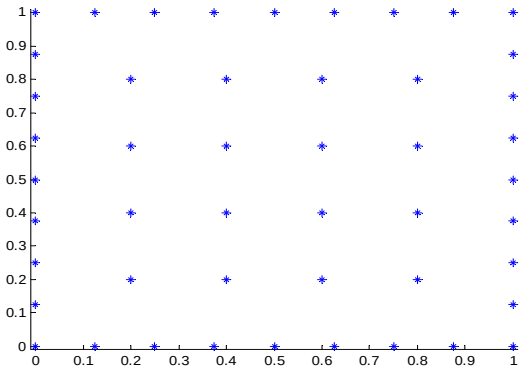

Figure 7.1: The distribution of collocation points for the RBF.

To verify the effectiveness of the MFS-RBF algorithm, we computed the errors at the point $(0.8, 0.8)$. The graph of $u(0.8, 0.8, t)$, for $0 \le t \le 25$, is shown in Figure 7.2. The errors using $\tau = 0.05$ and $\tau = 0.025$ are shown in Figure 7.3. Similar results were obtained at other points. The results are highly accurate for the smaller time step τ. Increasing the number of interpolation points from the current setting has little affect on the numerical accuracy. The numerical results using the MFS-RBF algorithm are superior to those in [Ingber and Phan-Thien (1992)]. The convergence rate of the method using different time steps is shown in Figure 7.4.

Example 7.2 Consider the diffusion equation (7.1) with $f = 0$ in a cubic region $0 \le x_1, x_2, x_3 \le 1$ with unit thermal conductivity and diffusivity. The boundary conditions are given by

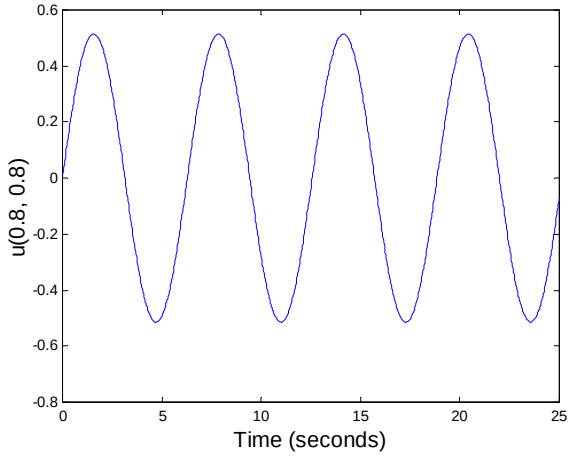

Figure 7.2: Profile of the solution of $u(0.8, 0.8, t)$ for $0 \le t \le 25$.

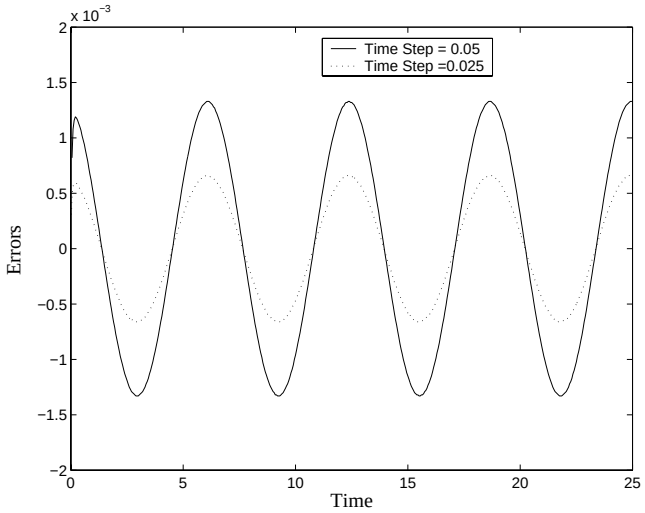

Figure 7.3: The profile of errors using $\tau = 0.05$ and $\tau = 0.025$ at $(0.8, 0.8)$.

$$u(0, x_2, x_3, t) = 0, u(1, x_2, x_3, t) = 1 \quad \text{for}$$
$$0 \le x_2, x_3 \le 1.0, \quad t > 0$$
$$\frac{\partial u}{\partial n}(x_1, x_2, 0, t) = \frac{\partial u}{\partial n}(x_1, x_2, 1, t) = 0 \quad \text{for}$$
$$0 \le x_1, x_2 \le 1.0, \quad t > 0,$$
$$\frac{\partial u}{\partial n}(x_1, 0, x_3, t) = \frac{\partial u}{\partial n}(x_1, 1, x_3, t) = 0 \quad \text{for}$$
$$0 \le x_1, x_3 \le 1.0, \quad t > 0.$$

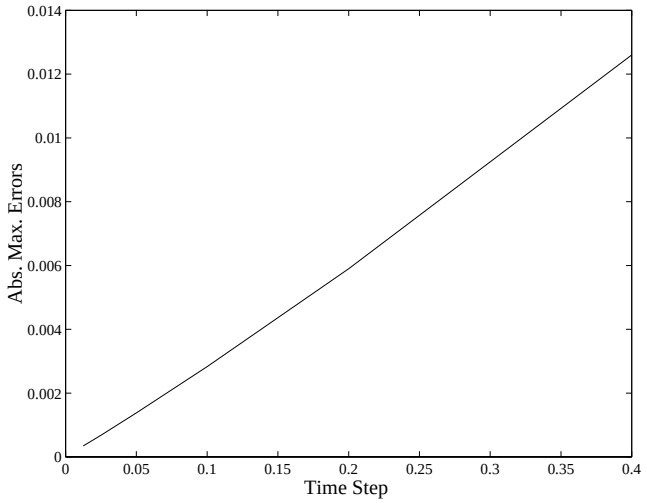

Figure 7.4: Convergence rate of the Euler method

The initial condition is given by $u(x_1,x_2,x_3,0) = 0$ for $0 < x_1,x_2,x_3 < 1$. This problem has been considered by [Ingber, Chen and Tanski (2004)]. It represents the 1D problem of an insulated unit bar with initial temperature zero whose left-hand boundary is isothermal at 0 and whose right hand boundary is impulsively raised to one at time $t = 0$. The exact solution can be determined using separation of variables and is given in [O'Neil (1999)].

The solution is discretized with 218 source points outside the domain ($M = 218$) and 343 interpolation points ($N = 343$). Among them, 218 of the interpolation points are located on the surface of the domain while the remaining 125 interpolation points are located in the interior of the domain. The radius of the fictitious boundary is 8. In Table 7.1, PS1, PS2 and PS3 denote polyharmonic splines $r^{2k-1}, k = 1,2,3$, respectively. In general, the results get better with higher order polyharmonic splines and reduced time steps, but this is not always the case. Care must be taken in either reducing the time step or going to higher order polyharmonic splines, since the higher-order polyharmonic splines result in worse conditioning of the linear system associated with the particular solution and smaller time steps result in worse conditioning (large λ) of the linear system associated with the homogeneous solution. In fact, for small time steps, the Euler implicit method ($\theta = 1$) is more accurate than the Crank-Nicolson method ($\theta = 0.5$) despite the difference in the local truncation error for the two methods. The current results are consistent with results of [Muleshkov, Golberg and Chen (1999)] who showed that improvement in accuracy can be obtained by using higher order polyharmonic splines for elliptic boundary value problems. Further, they show limited improvement for time-dependent problems presumably because the dominant error was caused by the time-stepping scheme.

Table 7.1: Absolute maximum errors at $t = 1$ using polyharmonic splines.

θ	Δt	PS1	PS2	PS3
	0.01	$1.00E-2$	$2.83E-3$	$1.38E-2$
	0.005	$1.57E-2$	$2.77E-3$	$2.40E-3$
0.5	0.002	$2.92E-2$	$2.47E-3$	$1.96E-3$
	0.001	$4.56E-2$	$2.50E-3$	overflow
	0.01	$1.73E-2$	$1.39E-2$	$1.38E-2$
	0.005	$1.35E-2$	$7.20E-3$	$7.07E-3$
1	0.002	$1.84E-2$	$3.31E-3$	$3.02E-3$
	0.001	$2.86E-2$	$2.26E-3$	$1.76E-3$

8 Conclusions

We have shown how to solve a class of second order time dependent PDEs in a mesh-free manner by converting IBVPs for these equations to solving a sequence of BVPs for inhomogeneous modified Helmholtz equations. These BVPs were solved by a combination of the method of particular solutions and Trefftz methods. The key ingredient in this approach is the need to compute a particular solution of the inhomogeneous modified Helmholtz equation. To do this, we focus on the DRM approach to obtain particular solutions based on radial basis function, polynomial or Fourier series approximations to the source term. The resulting homogenous BVP is then solved by either the MFS or the classical Trefftz bases obtained by separation of variables. The relation of these bases to the Bergman-Vekua integral operator method is discussed.

To satisfy the boundary conditions we considered using collocation, least squares and Galerkin's method. An important issue here is the problem of mitigating the ill-conditioning of the resulting linear system. Here, we proposed a number of techniques from the statistical literature based primarily on the SVD of the boundary matrices. This topic will be further investigated in future work. Some numerical results are presented using the MFS-RBF algorithm showing the accuracy of the method

for both two dimensional and three dimensional problems for transient heat conduction.

Although this approach appears quite promising, much remains to be done. One needs to determine optimal combinations of time removal schemes, source term approximation and Trefftz bases. Mitigating ill-conditioning and obtaining error estimates will be the focus of future work. Finally, exploiting additional structure such as axisymmetry is an important topic for future research.

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