Chapter 2

Initial and Two-Point Boundary Value Problems

In this chapter, we first review the basic mathematical background of finite difference approximations to initial and two-point boundary value problems which are related to flow problems in primitive variable, and stream function-vorticity forms. These results are then extended to two dimensional flow problems.

2.1 First Order System

We first consider a system of first order ordinary differential equations due to its close relation to the Navier-Stokes equations written in the primitive variable formulation.

2.1.1 Initial Value Problems (IVPs)

We consider the initial value problem:

\[ Du = f, \quad x \geq 0, \]  
\[ u(0) = \alpha. \]  

(2.1)

(2.2)

where \( u \) is a known vector \( (u_1, u_2, \ldots, u_n)^T \), \( f \) is a given vector \( (f_1, f_2, \ldots, f_n)^T \), and \( \alpha = (\alpha_1, \alpha_2, \ldots, \alpha_n)^T \) is also given. This system can be solved by many schemes of varying order. We have a particular interest in solving it by centered differences, because that is the usual method employed in solving the Navier-Stokes equations in primitive variable form.
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We first introduce some notation. The difference operators $D_0$, $D_+$, and $D_-$ are defined as:

\[
D_0 f_i = f_{i+1} - f_{i-1}, \quad D_+ f_i = f_{i+1} - f_i, \quad D_- f_i = f_i - f_{i-1},
\]

(2.3)

where $f_i = f(x_i)$ and $D_h$ will be used if we do not specify 0, + or −.

When a centered difference formula is used to approximate the first-order derivative, the system (2.1)-(2.2) becomes:

\[
\frac{1}{2h} D_0 u_i = f_i, \quad x_i = (i-1)h, \quad i = 1, 2, \ldots,
\]

(2.4)

\[
u_1 = \alpha,
\]

(2.5)

where $h$ is the uniform mesh size. The system (2.4) - (2.5) is not determined, and a second condition has to be provided by apply the differential equation (2.1) at $x = 0$ using a difference scheme other than centered differences. This is a quite standard approach in the literature.

However, if we check this approach carefully, we find that the reason a second condition is needed is that the centered difference does not connect neighbouring points. There are two sets of grid point where the solution is isolated. A connection between these two sets has to be provided to obtain a correct solution, and this is done in the standard approach by providing a second initial condition at $x = 0$. Actually, this connection need not be at $x = 0$, but could be anywhere in the domain. We denote the condition which will provide this connection as the necessary constraint. This observation can be generalized in the following statement:

**Statement 2.1** The system (2.1)-(2.2) can be discretized by a centered difference scheme if there is a necessary constraint between neighbouring points. The constraint can come from either:
1. discretizing equation (2.1) at $x = 0$ by any difference scheme other than the centered difference, or

2. discretizing equation (2.1) at any location $x$ by any difference scheme other than a centered difference.

The scheme is second-order accurate if the constraint also has second-order accuracy.

2.1.2 Two-Point Boundary Value Problems for a Two-equation System

We consider a system of two equations with separated boundary conditions which is related to Navier-Stokes type equations. The system is:

$$\begin{align*}
Du &= f, \quad 0 \leq x \leq 1, \\
u^1(0) &= \alpha, \quad u^1(1) = \beta,
\end{align*}$$

(2.6)

(2.7)

where $u = (u^1, u^2)^T$, and $f = (f^1, f^2)^T$. The centered difference approximation of system (2.6) - (2.7) is

$$\begin{align*}
\frac{1}{h} D_0 u_i &= f_i, \quad x_i = (i - 1)h, \quad i = 1, \ldots, N, \\
u^1_i &= \alpha, \quad u^1_N = \beta.
\end{align*}$$

(2.8)

(2.9)

Usually, the system has a unique solution when it is coupled, i.e., when $f$ is a function of both dependent variables $u^1$ and $u^2$. Thus the necessary constraints needed to connect the neighbouring points are not necessarily derived from both equations. The constraints can be obtained from one equation only for both dependent variables. This is summarized in the following statement:

**Statement 2.2** The system (2.8)-(2.9) becomes a determined system when constraints for each variable $u^1$ and $u^2$ are given. The constraints can be provided for both variables $u^1$ and $u^2$ either by applying
1. the differential equation for $u^2$ at both boundaries, or

2. a difference scheme other than centered differences at two points inside the domain.

2.1.3 One Dimensional Navier-Stokes Type Equations

The two-equation system we consider here is a direct analogue of the two dimensional Navier-Stokes equations [39]:

\[-DP + g + D^2u = 0,\]  \hspace{1cm} (2.10)

\[Du = f, \quad 0 \leq x \leq 1,\]  \hspace{1cm} (2.11)

\[u(0) = \alpha, \quad u(1) = \beta.\]  \hspace{1cm} (2.12)

There is no boundary condition given for $p$. This means that $p$ is only determined to within a constant. A compatibility condition, the integral constraint $\beta = \int_0^1 f dx + \alpha$, must also be satisfied.

The solution $(u_e, p_e)$ of equations (2.10) and (2.11) can be found by integration:

\[u_e = \alpha + \int_0^x f(x) dx, \quad p_e = p_0 + \int_0^x (g + D^2 u) dx,\]

where $p_0$ is a constant. Hence equations (2.10) and (2.11) have a unique solution if $p_0$ is given. We now consider the determined system:

\[-DP + g + D^2u = 0,\]  \hspace{1cm} (2.13)

\[Du = f, \quad 0 \leq x \leq 1,\]  \hspace{1cm} (2.14)

\[u(0) = \alpha, \quad \int_0^1 p dx = \gamma.\]  \hspace{1cm} (2.15)

The integral relation will determine the constant $p_0$. The discretized form of this system by centered difference is:

\[-\frac{1}{2h} D_0 p_i + g_i + \frac{1}{h^2} D_+ D_- u_i = 0,\]  \hspace{1cm} (2.16)
\[
\frac{1}{2h} D_0 u_i = f_i, \quad i = 2, \ldots, N - 1, \\
u_0 = \alpha, \quad \sum_{i=1}^{N} a_ip_i = \gamma.
\] (2.17)  
(2.18)

As in the two-point BVPs, the difference system is not determined unless two constraints for \( u_i \) and \( p_i \) are provided. The following statement proposes a way to impose the necessary constraints:

**Statement 2.3** The system (2.16)-(2.18) becomes a determined system when the constraints for each variable \( p_i \) and \( u_i \) are provided by applying,

1. the differential equation (2.18) at both boundaries, or
2. a difference scheme other than centered differences for equation (2.18) at two points inside the domain.

### 2.1.4 One Dimensional Poisson Type Equations

Instead of solving system (2.10)-(2.12) one can obtain a new equation for \( p \) by taking the derivative of equation (2.10), and using equation (2.11):

\[
D^2 p = Dg + D^2 f.
\] (2.19)

Condition (2.19) now replaces equation (2.11) in the system (2.10)-(2.12). This is frequently used in the numerical simulation of incompressible flow problems in two dimension, and is known as the pressure Poisson equation approach.

The equivalence of equations (2.11) and (2.19) is now ensured if and only if \( Du = f \) is imposed at some point in the domain. However, the enforcement of \( Du = f \), which we call the necessary constraint for the Poisson type approach, need not be on the boundary, but can be applied anywhere inside the domain. Then the equivalent system to (2.10)-(2.12)
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is

\[ -Dp + g + D^2u = 0, \quad (2.20) \]

\[ D^2p = Dg + D^2f_i, \quad 0 \leq x \leq 1, \quad (2.21) \]

\[ u(0) = \alpha, \quad u(1) = \beta, \quad (2.22) \]

\[ Du = f, \quad \text{some } x_c \in [0, 1], \quad \int_0^1 p \, dx = \gamma. \quad (2.23) \]

The integral relation will determine the integration constant for \( p \). The corresponding discrete form is

\[ -\frac{1}{2h} D_0 p_i + g_i + \frac{1}{h^2} (D_+ D_- u_i) = 0, \quad (2.24) \]

\[ D^2 p_i = Dg_i + D^2 f_i, \quad i = 2, \ldots, N - 1, \quad (2.25) \]

\[ u_0 = \alpha, \quad u_N = \beta, \quad (2.26) \]

\[ \frac{1}{2h} D_0 u_i = f_i, \quad \text{some } i \in [1, N], \quad \sum_{i=1}^{N} a_i p_i = \gamma. \quad (2.27) \]

Note that equations (2.25) is obtained from the discretized form of equation (2.20) and not directly from equation (2.21). This point will be discussed further for the two-dimensional case.

The type of approach will be determined by the chosen value \( x_c \), and the corresponding index \( i \). The discrete system (2.24)-(2.27) is not determined unless necessary constraints are imposed on \( u \) and \( p \). This is summarized in the following statement:

**Statement 2.4** The system (2.24)-(2.27) becomes a determined system which is the equivalent discrete form of (2.10)-(2.12) when the constraints for \( p \) and \( u \) can be provided by applying either:

1. the differential equation (2.20) at both boundaries, or

2. a difference scheme other than centered differences for equation (2.20) at two points inside the domain.
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The constraints needed to obtain a determined discretized system can be divided into two types: Boundary Constraints (BC) and Interior Constraints (IC). Although this is quite obvious now for one dimensional model problems, it is not quite as obvious in higher dimensional cases. Some of the methods proposed in the literature fail to provide such constraints, resulting in inaccurate solutions or failed to obtain a convergent solution (details will be given in discussion for two dimensional flow problems). Previous methods in the literature fit into the first catalog, the BC method. The IC method, which provides the necessary constraints without introducing extra information on the boundary, is favoured in this thesis.

2.2 Second Order System

In this section, the two-point boundary value problem for a system of two second order ordinary differential equations is discussed. Higher order system have a corresponding first system. However, we will discuss the second order system directly because of its relation to the Navier-Stokes equations in stream function-vorticity form in two dimensional case. The model problem is a system of two second-order equations for two dependent variables $\psi$ and $\zeta$, which has been used by Dennis and Quartapelle[55]. We write

\begin{align}
D^2\zeta + g(x, \psi) \cdot D\zeta &= f(x, \psi), \\
D^2\psi &= -\zeta, \quad 0 \leq x \leq 1,
\end{align}

with boundary conditions for one variable $\psi$ only:

\begin{align}
\psi(0) = \psi(1) &= 0, \quad D\psi(0) = D\psi(1) = 0,
\end{align}

where $D$ and $D^2$ denote first and second order derivatives with respect to $x$. The functions $f$ and $g$ could either be given function of $x$ or depend on $\psi$, in which case the problem...
is nonlinear. No explicit boundary conditions are given for the variable \( \zeta \), while the boundary conditions for \( \psi \) are overspecified.

The differential system (2.28)-(2.30) is a determined system in the sense that four boundary constraints are given for two second order differential equations. However, when a standard finite difference approach is used, the system is discretized as

\[
\frac{1}{h^2} D_+ D_- \zeta_i + g_i \cdot \frac{1}{2h} D_0 \zeta_i = f_i, \quad (2.31)
\]

\[
\frac{1}{h^2} D_+ D_- \psi_i = -\zeta_i, \quad x_2 \leq x_i \leq x_{N-1}, \quad (2.32)
\]

\[
\psi_1 = \psi_N = 0, \quad D_h \psi_1 = D_h \psi_N = 0. \quad (2.33)
\]

The difference system (2.31)-(2.33) is not determined in the usual sense, because no boundary conditions are available for \( \zeta \) on the physical boundaries, \( x_1(= 0) \) and \( x_N(= 1) \). However, if the discretization of the differential equation for \( \zeta \) at the physical boundaries is considered as the boundary condition for \( \zeta \), it overdetermines the system. Here we refer to the physical domain and the physical boundary as those for the original differential equations.

### 2.2.1 Woods Method

From Taylor expansion and the condition (2.33), we have

\[
\psi_2 = \sum_{i=0}^{\frac{3}{i!}} \frac{h^i}{i!} \psi_1^i + O(h^4), \quad \psi_{N-1} = \sum_{i=0}^{\frac{3}{i!}} \frac{(-h)^i}{i!} \psi_N^i + O(h^4). \quad (2.34)
\]

If \( D^2 \psi \) is substituted into equation (2.29) and discretized, boundary conditions are obtained for the variable \( \zeta \) as

\[
\zeta_1 = -\frac{3}{h^2} \psi_2 - \frac{1}{2} \zeta_2, \quad \zeta_N = -\frac{3}{h^2} \psi_{N-1} - \frac{1}{2} \zeta_{N-1}. \quad (2.35)
\]
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There are two steps involved here: the equation is imposed at the boundary and the variable \( \psi \) is expanded at the boundary. This becomes complicated in two dimensional cases with irregular boundary configurations.

2.2.2 Integral Constraint Method

By integrating equations (2.29) with weight functions \( \omega_i(x) \), we have

\[
\int_0^1 \zeta \omega_i dx = - \int_0^1 \omega_i D^2 \psi dx, \quad i = 1, 2. \tag{2.36}
\]

If we choose the weight functions to be \( \omega_1(x) = 1 \) and \( \omega_2(x) = x \), we have two equations for \( \zeta \):

\[
\int_0^1 \zeta dx = 0, \quad \int_0^1 x \zeta dx = 0. \tag{2.37}
\]

The equations in (2.37) are discretized and two global constraints for \( \zeta_1, \zeta_N \) are obtained.

In two dimensional situations, the area integral can be transformed to a boundary integral by Green’s theorem and a similar but more complicate formula can be obtained.

2.2.3 Influence Matrix Method

The linear system obtained by setting \( f(x, \psi) = f(x) \) and \( g(x, \psi) = g(x) \) is used to illustrate the idea of the influence matrix method. The equation (2.28) can be decomposed into three systems:

\[
D^2 \zeta_a + g \cdot D \zeta_a = -f, \quad D^2 \psi_a = -\zeta_a, \tag{2.38}
\]

\[
\psi_a(0) = \psi_a(1) = 0, \quad \zeta_a(0) = \zeta_a(1) = 0; \tag{2.39}
\]

and

\[
D^2 \zeta_+ + g \cdot D \zeta_+ = -f, \quad D^2 \psi_+ = -\zeta_+, \tag{2.40}
\]

\[
\psi_+(0) = \psi_+(1) = 0, \quad \zeta_+(0) = 0, \quad \zeta_+(1) = 1; \tag{2.41}
\]
and
\[ D^2 \zeta_- + g \cdot D \zeta_- = -f, \quad D^2 \psi_- = -\zeta_-, \quad (2.42) \]
\[ \psi_-(0) = \psi_-(1) = 0, \quad \zeta_-(0) = 1, \quad \zeta_-(1) = 0. \quad (2.43) \]

With \( \alpha_+ \) and \( \alpha_- \) as two constants to be determined, the superposition \( \zeta = \zeta_0 + \alpha_+ \zeta_+ + \alpha_- \zeta_- \) and \( \psi = \psi_0 + \alpha_+ \psi_+ + \alpha_- \psi_- \) are solutions of system (2.28)-(2.29). Then two linear constraints for \( \alpha_+ \) and \( \alpha_- \), known as the influence matrix, are obtained by satisfying the boundary conditions (2.30). The system (2.28)-(2.29) can be solved if the values of \( \alpha_+ \) and \( \alpha_- \) are determined. For the nonlinear case, the system is linearized first, and an iterative procedure is then used. A similar procedure can be used for two dimensional problems with, however much greater computational effort is needed for the calculation of such a system.

### 2.2.4 Interior Constraint Method

It can be seen that the basic idea of the methods discussed is to obtained a constraint between the \( \zeta \) boundary value and the over-specified boundary condition for \( \psi \). It is, however, not necessary to obtain such a constraint for the boundary value of \( \zeta \). From the mathematical point of view, \( \zeta \) is only an intermediate variable for obtaining a solution of \( \psi \). A fourth order equation for \( \psi \) can be obtained by eliminating \( \zeta \) from the system (2.28)-(2.29) as
\[ D^4 \psi + g(x, \psi) \cdot D^3 \psi = -f(x, \psi). \quad (2.44) \]

Equation (2.44) with boundary conditions (2.28) will be a determined system. The discretized system
\[ \frac{1}{h^4} D_+ D_- D_+ D_- \psi_i + \frac{1}{2h^3} g_i D_+ D_- D_0 \psi_i = -f_i \quad (2.45) \]
can be obtained directly from the discretized system (2.31)-(2.32). A relative full matrix system results from this discretization and special techniques are needed to solve this
system in the two dimensional case [51] since the usual procedure is unstable [50]. If we check this procedure carefully, we will find that there is no need to calculate the boundary values \( \zeta_1 \) and \( \zeta_N \). As a intermediate variable, only interior values \( \zeta_i \) \((i = 2, \ldots, N - 1)\) are used. Thus, if we prefer to solve the system (2.31)-(2.32) instead of the biharmonic equation (2.45), we still don’t need to calculate the intermediate variable, or ‘constraint’ \( \zeta_i \), on the boundary. The ‘constraint’ \( \zeta_i \) is only need to be provided in interior points. We call this approach the Interior Constraint (IC) method.

The basic idea of the IC method is the use of the implicit boundary conditions (2.33) as equations for the discretized variable \( \psi_i \) next to the boundary without using any information from \( \zeta_i \) on that grid. The \( \zeta_i \) variable at the same grid then can be obtained from equation (2.32) instead of equation (2.31). The system (2.31)-(2.32) with the boundary conditions (2.33) is now determined by this arrangement as:

\[
\frac{1}{h^2} D_+ D_- \zeta_i + \frac{1}{2h} g_i \cdot D_0 \zeta_i = f_i, \tag{2.46}
\]

\[
\frac{1}{h^2} D_+ D_- \psi_i = -\zeta_i, \quad x_3 \leq x_i \leq x_{N-2}, \tag{2.47}
\]

\[
D_h \psi_1 = D_h \psi_N = 0, \tag{2.48}
\]

\[
\zeta_2 = -\frac{1}{2h} D_+ D_- \psi_2, \quad \zeta_{N-1} = -\frac{1}{2h} D_+ D_- \psi_{N-1}, \tag{2.49}
\]

as equations at interior points and

\[
\psi_1 = \psi_N = 0, \tag{2.50}
\]

are the only boundary conditions needed. If the \( \zeta \) value at a boundary is required, as in physical problems, it can be obtained by apply equation (2.31) after the interior value is computed.

In the IC method, a computational domain is set up inside the physical domain. First, a mesh system with uniform grid size \( h \) and nodes \( x_i = (i - 1)h, i = 1, \ldots, N \), is
set up on the physical domain, $0 \leq x \leq 1$. The domain from $x_2$ to $x_{N-1}$ is now defined as the computational domain $\Omega^c$, i.e., one grid size into the physical domain $\Omega$, and the computational boundary $\partial \Omega^c$ is also moved one grid size in to $x_2$ and $x_{N-1}$. This is shown in Figure 2.1. $\Omega^c$ is related to a particular mesh, and approaches $\Omega$ when the mesh size approaches zero (Figure 2.1).

As a summary, the IC method produces a determined system by providing the necessary constraints on $\partial \Omega^c$. Besides the advantages of the simplicity and consistency in the discretization, the IC method is expected to introduce less error than other methods if there is a large variation in the solution near the boundary.