

CHAPTER II

MATHEMATICAL BACKGROUND

In this chapter, we will introduce some background knowledge of numerical simulation. The basic ideas of BEM and meshless method are briefed. Some general features of the meshless method are described.

2.1 Gaussian integration

To approximate the definite integration $\int_a^b f(x)dx$, we can change variable using a linear transformation as Figure 2.1

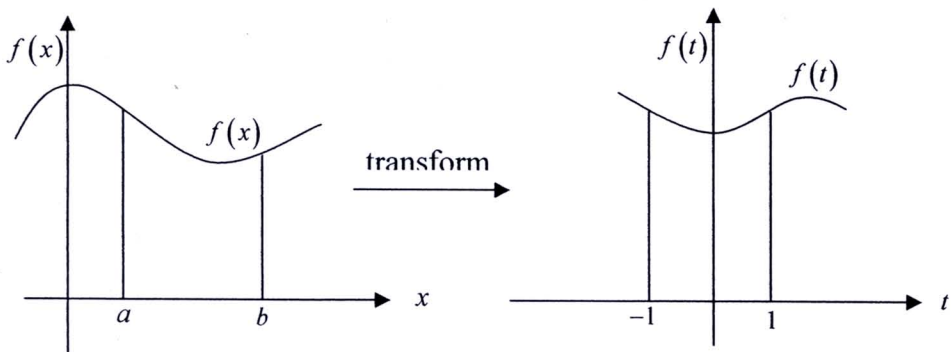


Figure 2.1 Transformation from the domain $a < x < b$ to $-1 < t < 1$

Suppose that

$$x = At + B \quad A, B \in \mathbb{R} \quad (2.1)$$

Assuming

$$x = a \quad \text{where} \quad t = -1 \quad (2.2)$$

$$x = b \quad \text{where} \quad t = 1$$

we obtain the system of linear equations as

$$x = A(-1) + B \quad (2.3)$$

$$x = A(1) + B \quad (2.4)$$

Solving (2.3) and (2.4), we obtain

$$A = \frac{b-a}{2}$$

$$B = \frac{b+a}{2}$$

In equation (2.1), we obtain

$$x = \frac{b-a}{2}t + \frac{b+a}{2} \quad \text{and} \quad dx = \frac{b-a}{2}dt$$

Thus

$$\begin{aligned} \int_a^b f(x) dx &= \int_{-1}^1 f\left(\frac{b-a}{2}t + \frac{b+a}{2}\right) \left(\frac{b-a}{2}\right) dt \\ &= \frac{b-a}{2} \int_{-1}^1 f\left(\frac{b-a}{2}t + \frac{b+a}{2}\right) dt \end{aligned} \quad (2.5)$$

The integral on the right hand side is approximated by using Gauss Quadrature as

$$\int_{-1}^1 f(t) dt \approx \sum_{k=1}^N f(t_k) w_k \quad (2.6)$$

where N is the number of Gauss integration point, t_k are the zeros of the Legendre polynomial

$$P_N(t) = \frac{1}{2^N N!} \frac{d^N}{dt^N} (t^N - 1)^N \quad (2.7)$$

and w_k are Gaussian weights given by the following formula

$$w_k = \frac{2(1-t_k^2)}{N^2 [P_{N-1}(t_k)]^2} \quad (2.8)$$

where the function in (2.6) is actually approximated by a polynomial of degree $2N-1$.

Therefore, rewritten (2.5) we obtain

$$\int_a^b f(x) dx \approx \frac{b-a}{2} \sum_{k=1}^N w_k f(t_k) \quad (2.9)$$

Table 2.1 provides the coordinates of the integration points and the weights for various values of N .

Table 2.1 Point and Gaussian weights

n	$x_{n,k}$	$w_{n,k}$
2	-0.5773502692	1.0000000000
	0.5773502692	1.0000000000
3	0.7745966920	0.5555555556
	0.0000000000	0.0000000000
	0.7745966920	0.5555555556
4	0.8611363446	0.3472518451
	-0.8611363446	0.3472518451
	0.3399810436	0.6521451549
	-0.3399810436	0.6521451549

2.2 Potential problem

A scalar function ϕ , defined on a domain Ω bounded by a closed cover $\partial\Omega$ or Γ , is a harmonic function if it is a solution of the Laplace equation

$$\nabla^2 \phi = 0 \quad (2.10)$$

Suppose that u is a harmonic function, i.e.

$$\nabla^2 u = 0 \text{ in } \Omega \quad (2.11)$$

and subject to the Dirichlet condition

$$u = \bar{u} \quad \text{on } \Gamma_1 \quad (2.12)$$

and the Neumann condition

$$\frac{\partial u}{\partial n} = q = \bar{q} \quad \text{on } \Gamma_2 \quad (2.13)$$

where n is a unit outward normal vector to the boundary

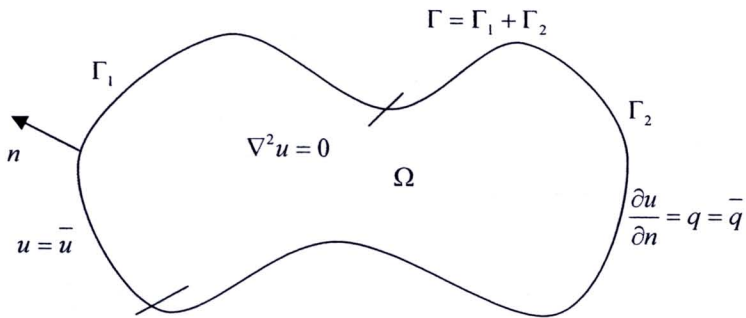


Figure 2.2 Laplace equation posed on the domain Ω with the boundary Γ

The combination of Laplace equation with this boundary condition is called Potential problem.

2.3 The divergence theorem

Let Ω be a regular domain with boundary Γ as shown in Figure 2.2 and let u be a vector function continuously differentiable at every point of Γ the divergence or the Gauss theorem states

$$\int_{\Omega} \nabla u d\Omega = \int_{\Gamma} u \cdot n ds \quad (2.14)$$

where n is the unit outward normal to the boundary.

2.4 Green's second identity

Suppose u and v are two functions defined in Ω bounded by the closed curve Γ . Assuming that they are continuous partial derivatives, from the basic property of the gradient, we have

$$\nabla \cdot (u \nabla v) = u \nabla^2 v + \nabla v \cdot \nabla u \quad (2.15)$$

$$\nabla \cdot (v \nabla u) = v \nabla^2 u + \nabla u \cdot \nabla v \quad (2.16)$$

Subtracting the two equations and integrating over Ω , we obtain

$$\int_{\Omega} (u \nabla^2 v - v \nabla^2 u) d\Omega = \int_{\Omega} \nabla \cdot (u \nabla v - v \nabla u) d\Omega \quad (2.17)$$

Applying the Gauss theorem (2.14) to the right hand side then gives

$$\int_{\Omega} \nabla \cdot (u \nabla v - v \nabla u) d\Omega = \int_{\Gamma} (u \nabla v - v \nabla u) \cdot n ds \quad (2.18)$$

Using the property of the gradient on the right hand side gives

$$\int_{\Omega} \nabla(u \nabla v - v \nabla u) d\Omega = \int_{\Gamma} \left(u \frac{\partial v}{\partial n} - v \frac{\partial u}{\partial n} \right) ds \quad (2.19)$$

Hence from (2.17) and (2.19) we obtain

$$\int_{\Omega} (u \nabla^2 v - v \nabla^2 u) d\Omega = \int_{\Gamma} \left(u \frac{\partial v}{\partial n} - v \frac{\partial u}{\partial n} \right) ds \quad (2.20)$$

This is the well-known second form of Green's theorem.

2.5 Laplace operator in polar coordinate

Let $u = u(x, y)$, $\vec{r} = x\vec{i} + y\vec{j}$, $r = |\vec{r}| = \sqrt{x^2 + y^2}$ and suppose that $x = r \cos \theta$, $y = r \sin \theta$.

We finally get an important equation expressed as

$$\begin{aligned} \nabla^2 u &= \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \\ &= \frac{\partial^2 u}{\partial r^2} + \frac{1}{r} \frac{\partial u}{\partial r} + \frac{1}{r^2} \frac{\partial^2 u}{\partial \theta^2} \end{aligned} \quad (2.21)$$

we note that if u depends only on r , we obtain

$$\nabla^2 u = \frac{\partial^2 u}{\partial r^2} + \frac{1}{r} \frac{\partial u}{\partial r} \quad (2.22)$$

2.6 The Dirac delta function

Consider the sequence of functions

$$f_k(x) = \begin{cases} \frac{k}{2}, & |x| < \frac{1}{k} \\ 0, & |x| \geq \frac{1}{k} \end{cases} \quad (2.23)$$

where k is a positive number.

We can see that

$$\int_{-\infty}^{\infty} f_k(x) dx = 1, \quad \forall k = 1, 2, 3, \dots$$

Let $\delta(x) = \lim_{k \rightarrow \infty} f_k(x)$ where $f_k(x)$ is the function with property (2.23). The function

$\delta(x)$ is known as delta function or Dirac delta function. In mathematics, the delta function is treated in the theory of generalizations as the definition below

$$\delta(x) = \begin{cases} 0; & x \neq 0 \\ \infty; & x = 0 \end{cases}$$

Let \bar{r}_0 be the position of P , $\bar{r} = \bar{r}_1 - \bar{r}_0$ and $r = |\bar{r}|$ and suppose that $u^*(r)$ is a fundamental solution of Laplace equation which satisfies

$$\nabla^2 u^*(r) + \delta(r) = 0 \quad (2.25)$$

where $\delta(r)$ is Dirac delta function.

We see that

$$\nabla^2 u^*(r) = 0 \quad (2.26)$$

everywhere except $r = 0$.

To find the fundamental solution, we first find the solution of the homogeneous equation (2.26). In polar coordinate

$$\nabla^2 u^*(r) = \frac{\partial^2 u^*}{\partial r^2} + \frac{1}{r} \frac{\partial u^*}{\partial r} + \frac{1}{r^2} \frac{\partial^2 u^*}{\partial \theta^2} \quad (2.27)$$

and since the solution depends only on r

$$\frac{d^2 u^*}{dr^2} + \frac{1}{r} \frac{du^*}{dr} = 0 \quad (2.28)$$

This can be solved analytically as

$$u^* = C \ln r + D \quad (2.29)$$

where C and D are constants. It is conventional to set $D = 0$.

Let Ω_ε be the disc bounded by the curve Γ_ε with center P and radius ε as shown in Figure 2.3. Integrating on Ω_ε of equation (2.25), we obtain

$$\int_{\Omega_\varepsilon} \nabla^2 u^*(r) dA = - \int_{\Omega_\varepsilon} \delta(r) dA \quad (2.30)$$

By the properties of Dirac delta function

$$\int_{\Omega_\varepsilon} \delta(r) dA = 1 \quad (2.31)$$

hence

$$\int_{\Omega_\varepsilon} \nabla^2 u^*(r) dA = -1 \quad (2.32)$$

Applying the divergence theorem, we have

$$\int_{\Omega_\varepsilon} \nabla^2 u^*(r) dA = \int_{\Omega_\varepsilon} \nabla \cdot (\nabla u^*(r)) dA = \int_{\Gamma_\varepsilon} \nabla u^*(r) \cdot n ds = \int_{\Gamma_\varepsilon} \frac{\partial u^*}{\partial n} ds \quad (2.33)$$

Taking partial derivative of (2.29)

$$\frac{\partial u^*}{\partial n} = C \cdot \frac{1}{r} \quad (2.34)$$

Substituting (2.34) in (2.33)

$$\int_{\Gamma_\varepsilon} \frac{\partial u^*}{\partial n} ds = \int_{\Gamma_\varepsilon} \frac{C}{r} ds = \int_0^{2\pi} \frac{C}{r} \cdot r d\theta = \int_0^{2\pi} C d\theta = 2\pi C \quad (2.35)$$

In equations (2.32) and (2.35), we obtain

$$C = -\frac{1}{2\pi}$$

Finally, we obtain the fundamental solution as

$$u^*(r) = -\frac{1}{2\pi} \ln r \quad (2.36)$$



In similarly way, in the 3-dimensions, the fundamental solution of Laplace equation is

$$u^*(r) = \frac{1}{4\pi r} \quad (2.37)$$

2.8 Basic integral equation for internal points

From Figure 2.3, applying the Green's second identity with $v = u^*$, we have

$$\int_{\Omega - \Omega_\varepsilon} (u \nabla^2 u^* - u^* \nabla^2 u) dA = \int_{\Gamma - \Gamma_\varepsilon} \left(u \frac{\partial u^*}{\partial n} - u^* \frac{\partial u}{\partial n} \right) ds \quad (2.38)$$

Since both u and u^* are harmonic functions in $\Omega - \Omega_\varepsilon$, the integral on the left hand side is zero, therefore

$$\begin{aligned} \int_{\Gamma - \Gamma_\varepsilon} \left(u \frac{\partial u^*}{\partial n} - u^* \frac{\partial u}{\partial n} \right) ds &= 0 \\ \int_{\Gamma} \left(u \frac{\partial u^*}{\partial n} - u^* \frac{\partial u}{\partial n} \right) ds &= - \int_{\Gamma_\varepsilon} \left(u \frac{\partial u^*}{\partial n} - u^* \frac{\partial u}{\partial n} \right) ds \end{aligned} \quad (2.39)$$

Substituting the fundamental solution u^* , $\frac{\partial u^*}{\partial n} = q$ and also taking limit as $\varepsilon \rightarrow 0$, we

have

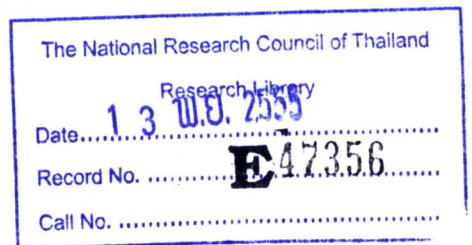
$$\int_{\Gamma} \left(u \frac{\partial}{\partial n} \left(-\frac{1}{2\pi} \ln r \right) - \left(-\frac{1}{2\pi} \ln r \right) \frac{\partial u}{\partial n} \right) ds = - \lim_{\varepsilon \rightarrow 0} \int_{\Gamma_\varepsilon} \left(u \frac{\partial}{\partial n} \left(-\frac{1}{2\pi} \ln r \right) - \left(-\frac{1}{2\pi} \ln r \right) \frac{\partial u}{\partial n} \right) ds \quad (2.40)$$

$$\frac{1}{2\pi} \int_{\Gamma} \left(\frac{u}{r} + q \ln r \right) ds = - \lim_{\varepsilon \rightarrow 0} \frac{1}{2\pi} \int_{\Gamma_\varepsilon} \left(\frac{u}{r} + q \ln r \right) ds \quad (2.41)$$

In the limit as $\varepsilon \rightarrow 0$, since u is continuous partial derivative

$$u \rightarrow u_p$$

$$q \rightarrow q_p$$



Hence

$$\frac{1}{2\pi} \int_{\Gamma} \left(\frac{u}{r} + q \ln r \right) ds = -\frac{1}{2\pi} u_p \lim_{\varepsilon \rightarrow 0} \int_{\Gamma_{\varepsilon}} \frac{1}{r} ds - \frac{1}{2\pi} q_p \lim_{\varepsilon \rightarrow 0} \int_{\Gamma_{\varepsilon}} \ln r ds \quad (2.42)$$

Computing the integral to the right hand side and rearranging the equation we obtain

$$u_p = -\frac{1}{2\pi} \int_{\Gamma} \left(u \left(\frac{1}{r} \right) + q \ln r \right) ds \quad (2.43)$$

$$\text{or } u_p = \int_{\Gamma} \left(-u \left(\frac{1}{2\pi r} \right) + q \left(-\frac{\ln r}{2\pi} \right) \right) ds \quad (2.44)$$

$$\text{i.e. } u_p = \int_{\Gamma} (qu^* - uq^*) ds \quad (2.45)$$

2.9 Basic integral equation for boundary points

Suppose that P is a vertex of an angle α on the boundary Γ as shown in Figure 2.4

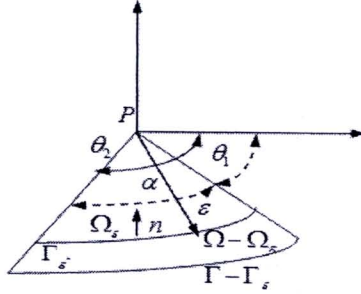


Figure 2.4 Domain with boundary point P

Applying the Green's second identity with $v = u^*$ to the region $\Omega - \Omega_{\varepsilon}$, where Γ_{ε} is the difference of Γ and Γ_{ε} , it follows that

$$\int_{\Omega - \Omega_{\varepsilon}} (u \nabla^2 u^* - u^* \nabla^2 u) dA = \int_{\Gamma - \Gamma_{\varepsilon}} \left(u \frac{\partial u^*}{\partial n} - u^* \frac{\partial u}{\partial n} \right) ds + \int_{\Gamma_{\varepsilon}} \left(u \frac{\partial u^*}{\partial n} - u^* \frac{\partial u}{\partial n} \right) ds \quad (2.46)$$

As in the previous section, the left hand side is zero, hence

$$\int_{\Gamma - \Gamma_{\varepsilon}} \left(u \frac{\partial u^*}{\partial n} - u^* \frac{\partial u}{\partial n} \right) ds = - \int_{\Gamma_{\varepsilon}} \left(u \frac{\partial u^*}{\partial n} - u^* \frac{\partial u}{\partial n} \right) ds \quad (2.47)$$

we will examine the integrals in the above equation when take $\varepsilon \rightarrow 0$, we have

$$\int_{\Gamma} \left(u \frac{\partial u^*}{\partial n} - u^* \frac{\partial u}{\partial n} \right) ds = -\lim_{\varepsilon \rightarrow 0} \int_{\Gamma_{\varepsilon}^-} u \frac{\partial u^*}{\partial n} ds + \lim_{\varepsilon \rightarrow 0} \int_{\Gamma_{\varepsilon}^+} u^* \frac{\partial u}{\partial n} ds \quad (2.48)$$

Computing the integral to the right hand side and using the fact that $\alpha = \theta_1 - \theta_2$, we obtain

$$-\frac{\alpha}{2\pi} u_p = \int_{\Gamma} \left(u \frac{\partial u^*}{\partial n} - u^* \frac{\partial u}{\partial n} \right) ds \quad (2.49)$$

Let $q^* = \frac{1}{2\pi r}$, $u^* = -\frac{1}{2\pi} \ln r$, so we get

$$C u_p = \int_{\Gamma} (u^* q - u q^*) ds \quad (2.50)$$

where $C = \frac{\alpha}{2\pi}$.

Equation (2.50) is known as the basic formula for the boundary element method. It is clear that if P is an interior point then $\alpha = 2\pi$ and hence $C = 1$. If P is a boundary point and the curve Γ is smooth, then $\alpha = \pi$ and $C = \frac{1}{2}$.

2.10 Radial basis functions (RBF)

Radial basis functions have been applied to solve many problems in science and engineering [31]. Over the past two decades radial basis functions have played an important role in the development of meshless method for solving PDEs [21, 33, 34, 35]. The following is a formal definition of a radial basis function.

Definition 1: A function $\Phi: \mathbb{R}^s \rightarrow \mathbb{R}$ with dimension s , is called radial basis function provided there exists a univariate function $\varphi: [0, \infty) \rightarrow \mathbb{R}$ such that $\Phi(x) = \varphi(r)$, where $r = \|x\|$, $x \in \mathbb{R}^s$, and $\|\cdot\|$ is some norm on \mathbb{R}^s —usually the Euclidean norm. In the following some of RBF are shown.

$$\varphi(r) = e^{-(\varepsilon r)^2} \quad \text{Gauss RBF.}$$

$$\varphi(r) = \frac{1}{\sqrt{1 + (\varepsilon r)^2}} \quad \text{Inverse multiquadric RBF (IMQ RBF).}$$

$$\varphi(r) = \sqrt{1 + (\varepsilon r)^2} \quad \text{Multiquadric.}$$

where $\varepsilon \geq 0$ are called shape parameter. Only Inverse multiquadric RBF is used for this work.

2.11 Scattered data interpolation

Given data $\{x_i, f_i\}$, $i = 1, \dots, N$, $x_i \in \mathbb{R}^s$ where $f_i(x) = f(x_i)$ and f is defined from a function $f: \mathbb{R}^s \rightarrow \mathbb{R}$. The formula for interpolation of a function P_f is defined by

$$P_f(x) = \sum_{j=1}^N c_j \varphi(\|x - x_j\|), \quad x \in \mathbb{R}^s \quad (2.51)$$

such that

$$P_f(x_i) = f(x_i), \quad i = 1, \dots, N. \quad (2.52)$$

c_j are coefficients to be determined and $\|x - x_j\|$ is Euclidean norm. In equation (2.51), φ is a radial basis function.

2.12 Generalized Hermite interpolation

We are given data $\{x_i, \lambda_i f\}$, $i = 1, \dots, N$, $x_i \in \mathbb{R}^s$ where $\lambda_i f(x) = \lambda f(x_i)$

$\Lambda = \{\lambda_1, \lambda_2, \dots, \lambda_N\}$ is linearly independent set of continuous linear functional, f is some data function, and we assume that the generalized Hermite interpolant is in the form

$$P_f(x) = \sum_{j=1}^N c_j \lambda_j^\xi \varphi(\|x - \xi_j\|), \quad x \in \mathbb{R}^s \quad (2.53)$$

and satisfying $\lambda_i P_f = \lambda_i f$, $i = 1, \dots, N$. (2.54)

λ^ξ denotes functional λ which acts on function φ , the function of the second argument ξ (see [12]).

The system of equations occurred from (2.53) is rewritten as

$$Ac = f_\lambda \quad (2.55)$$

which A has matrix entries as

$$A_{ij} = \lambda_i \lambda_j^\xi \varphi \quad i, j = 1, \dots, N \quad (2.56)$$

and

$$f_\lambda = [\lambda_1 f, \dots, \lambda_N f]^T.$$

2.13 Positive definite matrices

We note that the system occurred from previous interpolations can be written as

$$Ac = y$$

We know from linear algebra that this system will have a unique solution whenever the matrix A is non-singular. It is much better if we investigate the matrix A by considering positive definite matrices as the following definition.

Definition 2: A real symmetric matrix A is called positive semi-definite if its associated quadratic form is non-negative, i.e.

$$\sum_{j=1}^N \sum_{k=1}^N c_j c_k A_{jk} \geq 0 \quad (2.57)$$

for $c = [c_1, \dots, c_N]^T \in \mathbb{R}^N$.

If the quadratic form (2.57) is zero only $c \equiv 0$, then A is called positive definite. An important property of positive definite matrices is that all their eigenvalues are positive, and therefore a positive definite matrix is non-singular.

2.14 Halton points

Halton points (see [42, 43]) are created from *van der Corput sequences*. The starting point in the construction of a *van der Corput sequence* is the fact that every nonnegative integer n can be written uniquely using a prime base p , i.e.,

$$n = \sum_{i=0}^k a_i p^i \quad (2.58)$$

where each coefficient a_i is an integer such that $0 \leq a_i \leq p$. For example, if $n=10$ and $p=3$, then

$$10 = 1 \cdot 3^0 + 0 \cdot 3^1 + 1 \cdot 3^2$$

so that $k=2$ and $a_0 = a_2 = 1$ and $a_1 = 0$.

Next we define a function h_p that maps the nonnegative integers to the interval $[0,1)$ via

$$h_p(n) = \sum_{i=0}^k \frac{a_i}{p^{i+1}} \quad (2.59)$$

For example

$$h_3(10) = \frac{1}{3} + \frac{1}{3^3} = \frac{10}{27}.$$

The resulting sequence $h_{p,N} = \{h_p(n) : n = 0, 1, 2, \dots, N\}$ is called as a *van der Corput sequence*. For example

$$h_{3,10} = \{0, 1/3, 2/3, 1/9, 4/9, 7/9, 2/9, 5/9, 8/9, 1/27, 10/27\}.$$

In order to generate a Halton point set in s -dimensional space we take s primes p_1, \dots, p_s and use the resulting *van der Corput sequences* $h_{p_1,N}, \dots, h_{p_s,N}$ as the coordinates of the s -dimensional Halton points, i.e., the set

$$H_{s,N} = \{h_{p_1}(n), \dots, h_{p_s}(n) : n = 0, 1, 2, \dots, N\} \quad (2.60)$$

is the of $N+1$ Halton points in $[0,1]^s$.