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An Immersed Interface Method Algorithm
With Discontinuous Coefficients for the Energy equation

by

Hong Fang Zhu, B.Eng.

A thesis submitted to
the Faculty of Graduate Studies and Research
in partial fulfillment of the requirements for the degree of

Master of Engineering

Department of Mechanical and Aerospace Engineering

Ottawa-Carleton Institute for

Mechanical and Aerospace Engineering

Carleton University

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“An Immersed Interface Method Algorithm
With Discontinuous Coefficients For the Energy Equation”

submitted by Zhu Hong Fang, B.Eng.
in partial fulfilment of the requirements for
the degree of Master of Engineering

Thesis Supervisor
Dr. J. Goldak

Chair, Department
Dr. R. Bell

Carleton University

Abstract

The immersed interface method is used to derive numerical formulae for the Energy equation with discontinuous coefficients in one, two and three dimensions. The problem studied has an internal interface Γ in the domain Ω . The jump discontinuity in the temperature T is prescribed across Γ . The standard difference method is modified to produce second order accuracy on a uniform grid. This method is combined with different boundary conditions to develop an computer algorithm, which is used to simulate several steady state and transient problems.

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Variables List

α = a point on an interior interface.

φ = normal direction of the surface

θ = the angle between the x-axis and the normal direction of the surface

v = velocity.

H = enthalpy density.

Q = volumetric heat source.

q = flux of energy.

T = temperature.

h = contact conductance coefficient.

κ = conductivity coefficient.

C_p = specific heat per unit volume.

Δt = time step size.

d = mesh size .

ξ = tangential direction of the interface in $x - y$ plane.

η = normal direction of the interface in $x - y$ plane.

χ = normal direction of the interface in $x - y$ plane.

C_{ijk} = constant item.

n = time steps.

t = time step size.

v = Fourier number.

Chapter 1

Introduction

Many discontinuous problems arise in our physical world. One example is at the interface between two materials with different diffusion parameters in steady state heat diffusion. Another example is in electrostatic problems. In multicomponent flow problems, a Poisson problem with discontinuous coefficients also arises. Another example is the porous media equation used to model the interface between oil and a injected fluid in simulations of secondary recovery in oil reservoirs.

First, consider the energy conservation equation:

$$(1.1) \quad \dot{H} + \nabla \cdot q + Q = 0.$$

in a domain Ω , which is in one, two, or three space dimensions. Suppose there is an irregular surface interface within the domain, of which the function of temperature is known to be discontinuous across the interface. Assume that the domain is simple, such as a square in two dimensions, and we can use the standard finite difference method on a regular grid. The interface is typically not aligned with the grid, but cuts between grid points, so that for grid points near the interface, the stencil of a standard finite difference method will contain points from both sides of the interface. Because of the nonsmoothness of temperature, and the different values of temperature, the use of standard difference formulas will cause an incorrect approximation of the temperature. For discontinuities to arise in the solution or its derivatives there must be discontinuities or singularities present in the coefficients of the equation.

One possible solution was suggested by LeVeque[12] in 1994, and was used to solve the elliptic equation on a uniform grid in one or two di-

mensions. Usually the different kinds of the equations, say

$$(1.2) \quad a \frac{\partial^2 u}{\partial x^2} + b \frac{\partial^2 u}{\partial x \partial y} + c \frac{\partial^2 u}{\partial y^2} + d \frac{\partial u}{\partial x} + e \frac{\partial u}{\partial y} + f u + g = 0.$$

depends on the coefficient a, b, c , so if

$$b^2 - 4ac \leq 0.$$

the equation (1.2) is said to be an elliptic differential equation. An example is *Possion's equation*

$$\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = -g.$$

He derived appropriate coefficients at the grid points. He used a stencil that contains (in two dimensions) at most six points: the points of the standard five-point stencil plus a sixth point if we are near the interface. The sixth point is chosen from the set of diagonally adjacent grid points. The coefficients at these six points can be determined by solving a system of six linear equations.

1.1 The scope of the work

This present work will deal with the development of the analysis for solving the energy conservation equation with a temperature discontinuity across an interface in one dimension, two dimensions and three dimensions. The internal boundary may have any specified geometry provided that it is sufficiently smooth.

This work derives the appropriate approximation for the temperature jump using second order methods for the governing heat equation.

The analysis begins with an initial temperature in the different materials. The transient analyse is continued until steady state has been achieved.

Computer algorithms are developed to analysis the problem. The output from the computer program will provide the whole procedure for each time step of the temperature distribution in the different two parts, e.g., die and casting.

1.2 Objective of Thesis

The fundamental numerical formula to solve the heat equation with discontinuities in temperature for one dimensional and two dimensional space problems will be derived and the accuracy of the algorithms will be evaluated for several test cases.

Chapter 2

Literature Review

In 1960, Russian mathematicians Tikhonov and Samarskii [2] created the homogeneous difference scheme for one dimensional problems. It is suitable for transforming differential equations whose coefficients belong to certain class of function into difference equations. They also derived second-order accuracy on uniform grids with continuous and discontinuous conditions in the coefficients.

Mayo and GreenBaum [1] considered a similar problem in 1984 in two dimensions. They used rapid finite difference methods to solve Poisson's and biharmonic equation in irregular regions. The region was embedded in

a regular region where a fast solver can be used on a uniform grid and the right-hand side is appropriately modified near the original boundary. Also, they considered interface problems in magnetostatics with a piecewise constant coefficients.

In the early 70's, Peskin [3] approached a more complicated problem with similar characteristics in using the "immersed Boundary Method" to solve the incompressible Navier-Stokes equations in a region with complicated geometry. This method was originally used to model blood flow in the heart and for many other problems, particularly in biophysics. The idea is to solve Navier-Stokes equation on a uniform grid in a rectangular region in spite of complicated time-varying geometry, like a heart wall. The boundary can be viewed as moving with the velocity of the fluid and exerting force on the fluid. As a result, the normal derivative of the tangential velocity will typically have a jump discontinuity at the interface. But Peskin's approach for the Navier-stokes equations can be applied only to the elliptic equation with a delta function forcing term and in cases without discontinuous coefficients.

Based on Peskin's method, Beyer and LeVeque [10] modified Peskin's delta function and showed that second-order accuracy can still be obtained with an appropriate delta function in the time-dependent problem. But the problem appears that in two space dimensions, it does not reach second-order accuracy at all grid points.

2.1 LeVeque's immersed interface method for elliptic equations with discontinuous coefficients and singular sources

More recently, LeVeque and his co-researcher have developed a new method to extend their previous approach based on Peskin's method to deal with time-varying boundaries which produce second-order accuracy [12] in one and two dimensions with the jump condition.

2.1.1 One-dimensional problems

In the one dimensional problem, LeVeque considered the equation:

$$(2.1) \quad (\beta u_x)_x + \kappa u = f + C\delta(x - \alpha).$$

This problem was considered on the interval $[0, 1]$ with specified boundary conditions on u at $x = 0$ and $x = 1$. The function β could be discontinuous at $x = \alpha$, and u could also have a jump discontinuity at $x = \alpha$ of specified strength $\hat{C}$:

$$(2.2) \quad [u] = u^+ - u^- = \hat{C}.$$

Also, one could get the βu_x jump condition from equation (2.1).

One can approximate the solution $u(x)$ on a uniform grid in the interval $[0, 1]$, with

$$x_i = ih.$$

$$i = 1, 2, \dots, n.$$

where $h = 1/n$. The discontinuous point $x = \alpha$ usually falls between grid points, say $x_j \leq \alpha < x_{j+1}$. The goal is to develop finite difference equations of the form:

$$(2.3) \quad \gamma_{i,1}u_{i-1} + \gamma_{i,2}u_i + \gamma_{i,3}u_{i+1} + \kappa_i u_i = f_i + C_i.$$

There are two cases here: one is for $i \neq j, j+1$, where j and $j+1$ are the points between which the interface falls. The solution u is smooth in the interval $[x_{i-1}, x_{i+1}]$ and one can use the standard approximation. In this case, one can take:

$$\begin{aligned} \gamma_{i,1} &= \frac{\beta_{i-1/2}}{h^2} \\ \gamma_{i,2} &= -\frac{(\beta_{i-1/2} + \beta_{i+1/2})}{h^2} \\ \gamma_{i,3} &= \frac{\beta_{i+1/2}}{h^2}. \end{aligned}$$

and

$$C_i = 0.$$

This gives a local truncation error $O(h^2)$

$$(2.4) \quad T_i = \gamma_{i,1}u(x_{i-1}) + \gamma_{i,2}u(x_i) + \gamma_{i,3}u(x_{i+1}) + \kappa_i - f_i = O(h^2)$$

Another case is for $i = j, j + 1$, in which the jump condition is involved. In this case, one can also expand u_{i-1}, u_j and u_{j+1} in a Taylor's series about the point $x = \alpha$. The jump conditions are used to express all the terms in formula (2.4) in u^-, u_x^-, u_{xx}^- notation. The symbol “-” value represents values on the left side of the discontinuous point α . To ensure second order accuracy, all coefficients of u^-, u_x^-, u_{xx}^- must vanish, as well as the constant term. This will give four equations for the four unknown's $\gamma_{j,1}, \gamma_{j,2}, \gamma_{j,3}$ and C_j . From these simultaneous equations, one can obtain the unknown γ 's and the constant term C_j .

2.1.2 Two-dimensional problems

In two dimensions, the idea will be the same as for one dimension. The equation in two-dimensions is written as follows:

$$(2.5) \quad (\beta u_x)_x + \beta u_y)_y \kappa u = f(x, y) \quad (x, y) \in \Omega.$$

Here, assume that β is piecewise constant and has a jump discontinuity across some curve Γ in the domain Ω . In order to solve this equation, LeVeque took a uniform grid in the square domain Ω with

$$x_i = a + ih, \quad y_j = a + jh, \quad i, j = 0, 1, 2, 3, \dots, n.$$

where

$$h = (b - a)/n.$$

The goal here is to develop a finite difference equation of the form

$$(2.6) \quad \sum_k \gamma_k u_{i+i_k, j+j_k} + \kappa_{ij} u_{ij} = f_{ij} + C_{ij}.$$

The sum over k involves a finite number of points neighboring (x_i, y_j) (at most six in the formula derived). Since there is an interface in the domain Γ , LeVeque divided the solution into two cases.

1. The first is for regular points, where the interface does not come between any points in the standard five-point stencil centered at (i, j) . In this case, one can take

$$\gamma_1 = \gamma_3 = \gamma_4 = \gamma_5 = \frac{3}{h^2}$$

$$\gamma_2 = -\frac{43}{h^2}$$

and

$$\gamma_6 = 0.$$

2. Second, he considered irregular points for which the interface does come between some points in the standard five-point stencil centered at (i, j) . Following the same approach as in one dimension, expand the $u_{i+i_k, j+j_k}$ about some point (x_i^*, y_j^*) on the interface Γ .

The jump condition in two dimensions is:

$$(2.7) \quad u^- = u^+.$$

where we use the notation u^-, u^+ as follow:

$$u^- = \lim_{x \rightarrow \alpha^-} u(x).$$

$$u^+ = \lim_{x \rightarrow \alpha^+} u(x).$$

$$(2.8) \quad \beta^- \frac{\partial u^-}{\partial n} = \beta^+ \frac{\partial u^+}{\partial n}.$$

where $\partial/\partial n$ represents differentiation in the normal direction. and equation (2.7) gives information on the tangential direction. In order to eliminate the one side value, these jump conditions need to be manipulated. To do this, we can first perform a local coordinate trans-

formation into directions ξ normal to Γ and η . tangential to Γ .

In this way, the truncation error can be expressed as a linear combination of the values u^- , u_x^- , u_{xx}^- , u_y^- , u_{xy}^- and u_{yy}^- . To ensure second order accuracy in our numerical solution, all the coefficients of each of these terms should vanish. This will give a linear system of six equations to determine the coefficients γ_k . So LeVeque uses the standard five-point stencil together with one additional point. After getting all these coefficients and constant term C_j , the finite difference equation for point (x_i, y_j) can be used. For detail of the solution process reference may be made to Randall J. LeVeque and ZhuLin, Li (1994).

Chapter 3

Derivation of formulae

3.1 Introduction

The geometry of a transient heat transfer problem with a temperature discontinuity at a contact conductance is illustrated in Fig. (3.1). It shows one die section and one casting section. When modelling the problem, a contact conductance coefficient has been used, because air gap between the die and casting is so small compared to the size of a die or a casting. Although the heat flux is continuous near the contact, the temperature will have a jump at the gap if the flux is not zero.

Here LeVeque's embedded boundary volumetric method [12] is

Figure 3.1: Die Casting Model

applied to solve the following conservation of energy equation with a contact conductance and a discontinuous conductivity coefficients:

$$(3.1) \quad \dot{H} + \nabla \cdot q + Q = 0.$$

where

$$(3.2) \quad \dot{H} = \frac{DH}{Dt} = \frac{\partial H}{\partial t} + v \cdot \nabla H.$$

where v is velocity, H is enthalpy density, Q is a volumetric heat source (w/m^3) and q is the flux of energy.

At the air gap, the flux is considered to be continuous and the temperature is discontinuous. The jump of the temperature $[T]$ is

$$(3.3) \quad [T] = q/h.$$

where q is the heat flux and h is the contact conductance coefficient.

On the other hand, if $h = \infty$, the jump is zero. In this case, the temperature should be continuous, but the gradient of the temperature is not, because

$$(3.4) \quad q = \kappa \frac{\partial T}{\partial t}.$$

where κ is conductivity coefficient, T is the temperature and t is time.

In the die casting problems we are interested in, it is reasonable to assume the advective component of the material derivative (3.2) is negligible, since the velocity is zero. Also, in our case we just consider the energy equation without heat source, then formula (3.2) can be written as:

$$(3.5) \quad \frac{\partial H}{\partial t} + \nabla \cdot q = 0.$$

If we assume a linear relationship between enthalpy and temperature, then specific heat per unit volume (c_p) is constant. We can write the form (3.5) in terms of temperature as:

$$(3.6) \quad c_p \frac{\partial T}{\partial t} + \nabla \cdot q = 0.$$

3.2 One-dimensional problems

3.2.1 Numerical solution for one dimension

Let us begin with the one-dimensional form of (3.6):

$$(3.7) \quad c_p \frac{\partial T}{\partial t} + (-\kappa T_x)_x = 0.$$

Assume that at the point $x = \alpha$, a contact conductance exists, so that there will be a jump in the temperature across the position of discontinuity with specified strength $\hat{C}$.

$$(3.8) \quad [T] = T^+ - T^- = \hat{C}.$$

Across the point of discontinuity we have:

$$(3.9) \quad [q] = [\kappa T_x] = \kappa^+(T_x)^+ - \kappa^-(T_x)^-.$$

where

$$[q] = q^+ - q^- = 0.$$

Equations (3.8) and (3.9) provide constraints at $x = \alpha$.

We wish to approximate the solution $T(x)$ on a uniform grid in the interval $[0,1]$, with

$$x_i = id \quad i = 1, 2, 3 \dots n - 1 .$$

where $d = 1/n$. The point α typically falls between $x_j \leq \alpha \leq x_{j+1}$ for some j . Our goal is to develop the difference equation:

$$(3.10) \quad \gamma_{i,1}T_{i-1,t} + \gamma_{i,2}T_{i,t} + \gamma_{i,3}T_{i+1,t} = f(x,t) + C_i.$$

where γ 's are the coefficients of the equation to be determined, C_i is a constant term, and

$$f(x,t) = -c_p \frac{\partial T}{\partial t}.$$

(to simplify the equation (3.7)).

There are two cases to consider.

1. For $i \neq j, j + 1$, the solution is smooth in the interval $[x_{i-1}, x_{i+1}]$. and we can use the standard approximation

$$(3.11) \quad \frac{1}{d^2}(\kappa_{i+1/2}(T_{i+1,t} - T_{i,t}) - \kappa_{i-1/2}(T_{i,t} - T_{i-1,t})) = f(x,t).$$

$$\text{where } \kappa_{i+1/2} = \kappa(x_{i+1/2}), \quad f_i = f(x_i, t).$$

The truncation error here is defined as the difference between the approximate solution $T(x_j, t_n)$ and the exact solution $T(x, t)$ of the

differential equation. Usually, we use a Taylor's series expansion to express the exact solution as an infinite series. Therefore we can also use Taylor series expansions to express the truncation error.

In the case $(i \neq j, j + 1)$, we can take:

$$\begin{aligned}\gamma_{i,1} &= \frac{\kappa_{i-1/2}}{d^2} & \gamma_{i,2} &= \frac{-(\kappa_{i-1/2} + \kappa_{i+1/2})}{d^2} \\ \gamma_{i,3} &= \frac{\kappa_{i+1/2}}{d^2}\end{aligned}$$

and

$$C_i = 0.$$

Which gives a local truncation error is of order $O(d^2)$

$$\begin{aligned}t_i &= \gamma_{i,1}T(x_{i-1}, t) + \gamma_{i,2}T(x_i, t) + \gamma_{i,3}T(x_{i+1}, t) - f(x, t) \\ (3.12) \qquad \qquad \qquad &= O(d^2).\end{aligned}$$

2. For $i = j, j + 1$, (The nodes on either side of the interface. In one dimension, we just define the interface as the point α). where the jump exists. We still wish to determine the coefficients $\gamma_{i,1}, \gamma_{i,2}, \gamma_{i,3}$ and C_i

in equation (3.10), so that second order global accuracy is obtained.

To compute the local truncation error at the point x_j , we expand $T_{j-1,t}$, $T_{j,t}$, and $T_{j+1,t}$ in a Taylor series about the point $x = \alpha$. In order to ensure second order accuracy, we must expand through to $O(h^3)$.

$$\begin{aligned} T(x_{j-1}, t) = T^-(t) + (x_{j-1} - \alpha)T_x^-(t) + \frac{1}{2}(x_{j-1} - \alpha)^2T_{xx}^-(t) \\ + O(h^3). \end{aligned} \quad (3.13)$$

$$\begin{aligned} T(x_j, t) = T^-(t) + (x_j - \alpha)T_x^-(t) + \frac{1}{2}(x_j - \alpha)^2T_{xx}^-(t) \\ + O(h^3). \end{aligned} \quad (3.14)$$

$$\begin{aligned} T(x_{j+1}, t) = T^+(t) + (x_{j+1} - \alpha)T_x^+(t) + \frac{1}{2}(x_{j+1} - \alpha)^2T_{xx}^+(t) \\ + O(h^3). \end{aligned} \quad (3.15)$$

In order to eliminate the T^+ , T_x^+ , T_{xx}^+ from equation (3.13) to (3.15), we use the jump conditions (3.3):

$$T^+(t) = T^-(t) + \frac{q}{h} \quad . \quad (3.16)$$

where h is the contact conductance coefficient. we also have:

$$-\kappa^- T_x^-(t) = -\kappa^+ T_x^+(t),$$

or

$$(3.17) \quad T_x^+(t) = \frac{\kappa^-}{\kappa^+} T_x^-(t).$$

Equation $\kappa^- T_x^- = \kappa^+ T_x^+$ is continuous at $x = \alpha$ and we can differentiate it to get

$$\kappa_x^+ T_x^+(t) + \kappa^+ T_{xx}^+(t) = \kappa_x^- T_x^-(t) + \kappa^- T_{xx}^-(t).$$

Hence we obtain

$$(3.18) \quad T_{xx}^+(t) = \frac{\kappa^-}{\kappa^+} T_{xx}^-(t).$$

(because $\kappa_x^+ = \kappa_x^- = 0$)

Using these expressions in (3.15) gives

$$(3.19) \quad T(x_{j+1}, t) = T^- + \left((x_{j+1}(t) - \alpha) \left(\frac{\kappa^-}{\kappa^+} \right) + \frac{\kappa^-}{h} \right) T_x^- + \frac{\kappa^-}{2\kappa^+} (x_{j+1}(t) - \alpha)^2 T_{xx}^-(t).$$

To compute the local truncation error, we also use equation (3.7), and approach α from the left

$$(3.20) \quad \kappa_x^- T_x^-(t) + \kappa^- T_{xx}^-(t) = f(x, t).$$

We use this to replace the $f(x, t)$ term in the local truncation error and hence

$$(3.21) \quad \begin{aligned} t_j = & \gamma_{j,1} T(x_{j-1,t}) + \gamma_{j,2} T(x_{j,t}) + \gamma_{j,3} T(x_{j+1,t}) - [\kappa_x^- T_x^-(t) \\ & + \kappa^- T_{xx}^-(t)] - C_j. \end{aligned}$$

Replacing the $T(x_{j-1,t})$, $T(x_{j,t})$ and $T(x_{j+1,t})$ by Taylor's expansions (3.13) to (3.15) and collecting terms, gives

$$(3.22) \quad \begin{aligned} t_j = & (\gamma_{j,1} + \gamma_{j,2} + \gamma_{j,3}) T^-(t) + ((x_{j-1,t} - \alpha) \gamma_{j,1} + (x_{j,t} - \alpha) \gamma_{j,2} \\ & + \frac{\kappa^-}{\kappa^+} (x_{j+1,t} - \alpha + \frac{\kappa^-}{h}) \gamma_{j,3}) T_x^-(t) + (\frac{1}{2} \gamma_{j,1} (x_{j-1,t} - \alpha)^2 \\ & + \frac{1}{2} \gamma_{j,2} (x_{j,t} - \alpha)^2 + \frac{\kappa^-}{2\kappa^+} \gamma_{j,3} (x_{j+1,t} - \alpha)^2 - \kappa^-) T_{xx}^-(t) \\ & - C_j + O(d) \end{aligned}$$

To ensure that $t_j = O(d^2)$, we require that each coefficient of T^- , T_x^- , T_{xx}^- and the constant term vanish. This gives four equations for the four

unknowns $\gamma_{j,1}, \gamma_{j,2}, \gamma_{j,3}$ and C_j .

$$\gamma_{j,1} + \gamma_{j,2} + \gamma_{j,3} = 0$$

$$(x_{j-1,t} - \alpha)\gamma_{j,1} + (x_{j,t} - \alpha)\gamma_{j,2} + \frac{\kappa^-}{\kappa^+}(x_{j+1,t} - \alpha + \frac{\kappa^-}{h})\gamma_{j,3} = 0$$

$$\frac{1}{2}(x_{j-1,t} - \alpha)^2\gamma_{j,1} + \frac{1}{2}(x_{j,t} - \alpha)^2\gamma_{j,2} + \frac{\kappa^-}{2\kappa^+}(x_{j+1,t} - \alpha)^2\gamma_{j,3} = \kappa^-$$

and $C_j = 0$. Defining:

$$D_{j-1} = x_{j-1,t} - \alpha \quad D_{j+1} = x_{j+1,t} - \alpha. \quad D_j = x_{j,t} - \alpha$$

we can write the three equations in the matrix form

$$\begin{vmatrix} 1 & 1 & 1 \\ D_{j-1} & D_j & \frac{\kappa^-}{\kappa^+}D_{j+1} + \frac{\kappa^-}{h} \\ \frac{1}{2}D_{j-1}^2 & \frac{1}{2}D_j^2 & \frac{\kappa^-}{\kappa^+}D_{j-1}^2 \end{vmatrix} \begin{vmatrix} \gamma_{j,1} \\ \gamma_{j,2} \\ \gamma_{j,3} \end{vmatrix} = \begin{vmatrix} 0 \\ 0 \\ \kappa^- \end{vmatrix}$$

and solve for the γ 's at point j .

In a similar way, we can determine the coefficients in the equations at x_{j+1} from the system.

$$\gamma_{j+1,1} + \gamma_{j+1,2} + \gamma_{j+1,3} = 0$$

$$\left(-\frac{\kappa^+}{h} + \frac{\kappa^+}{\kappa^-}(x_{j,t} - \alpha)\right)\gamma_{j+1,1} + (x_{j+1,t} - \alpha)\gamma_{j+1,2} + (x_{j+2,t} - \alpha)\gamma_{j+1,3} = 0$$

$$\frac{\kappa^+}{2\kappa^-}(x_{j,t} - \alpha)^2\gamma_{j+1,1} + \frac{1}{2}(x_{j+1,t} - \alpha)^2\gamma_{j+1,2} + \frac{1}{2}(x_{j+2,t} - \alpha)^2\gamma_{j+1,3} = \kappa^+$$

or in matrix form:

$$\begin{vmatrix} 1 & 1 & 1 \\ \frac{\kappa^+}{\kappa^-}D_j - \frac{\kappa^+}{h} & D_{j+1} & D_{j+2} \\ \frac{\kappa^+}{2\kappa^-}D_j^2 & \frac{1}{2}D_{j+1}^2 & \frac{1}{2}D_{j+2}^2 \end{vmatrix} \begin{vmatrix} \gamma_{j+1,1} \\ \gamma_{j+1,2} \\ \gamma_{j+1,3} \end{vmatrix} = \begin{vmatrix} 0 \\ 0 \\ \kappa^+ \end{vmatrix}$$

$$\text{where } D_j = x_{j,t} - \alpha \quad D_{j+1} = x_{j+1,t} - \alpha \quad D_{j+2} = x_{j+2,t} - \alpha$$

These two systems have unique solutions unless the determinant of the matrix is zero. In which case the system of equations will be singular.

More generally, if $\kappa^+\kappa^- > 0^1$, it can be shown that the system of equations will have unique solutions for d sufficiently small, since the coefficients are almost constant in a neighborhood of the point α on a

¹In our physical problem, we will only consider κ^+, κ^- both positive

fine enough grid.

Now let us substitute $f(x, t)$ back to $c_p(\frac{\partial T}{\partial t})$. We obtain:

$$(3.23) \quad \gamma_{i,1}T_{i-1,t} + \gamma_{i,2}T_{i,t} + \gamma_{i,3}T_{i+1,t} = c_p \frac{(T_{i,t+1} - T_{i,t})}{\Delta t} \quad .$$

or

$$T_{i,t+1} = \frac{\Delta t}{c_p}(\gamma_{i,1}T_{i-1,t} + \gamma_{i,2}T_{i,t} + \gamma_{i,3}T_{i+1,t}) + T_{i,t}.$$

3.2.2 Numerical stability

In order to ensure the stability of the numerical solution in the explicit method that we are using right now, we need to satisfy the condition in the one dimensional case:

$$\Delta t \leq 0.5 \frac{d^2}{\nu}.$$

where

$$\nu = \frac{\kappa^{\pm}}{c_p^{\pm}}.$$

So

$$\Delta t \leq \min(0.5 \frac{c_p^+}{\kappa^+} d^2, \quad 0.5 \frac{c_p^-}{\kappa^-} d^2).$$

3.3 Two-dimensional problem

Now, we solve Equation (3.6) in two-dimensions

$$(3.24) \quad c_p \frac{\partial T}{\partial t} + (-\kappa T_x)_x + (-\kappa T_y)_y = 0 \quad (x, y) \in \Omega.$$

we assume κ is piecewise constant and has a jump discontinuity across some curve Γ in the domain Ω (Γ will referred to as the interface.) . Instead of one point as in a one dimensional problem, the interface Γ can be arbitrary piecewise smooth curve in Ω . It can be a closed or open curve. As for one dimension, we consider the temperature jump across the discontinuity to satisfy

$$[T] = q/h.$$

and also the flux is assumed to be continuous across discontinuity.

To simplify the problem, we make the the assumption that the domain Ω is a square, say $[a, b] \times [a, b]$. We take a uniform grid with

$$x_i = a + id, \quad y_j = a + jd, \quad i, j = 0, 1, \dots, n.$$

where $d = (b - a)/n$.

Similar to the one dimensional problem, our goal is to develop a finite difference equation of the form

$$(3.25) \quad \sum_k \gamma_k T_{i+i_k, j+j_k} = f_{ij} + C_{ij}.$$

for the point (x_i, y_j) . The sum over k involves a finite number (at most six points) of points neighboring (x_i, y_j) . So each i_k, j_k will take values in the set $\{-1, 0, 1\}$. The coefficients γ_k and i_k, j_k will depend on (i, j) . As in the one-dimensional problem, there are two cases to consider here too.

3.3.1 Numerical solution in two dimensions

1. We define a *regular point* as a point (i, j) such that the interface does not come between any points in the standard five-point stencil centered at (i, j) . We may use the standard five-point finite difference scheme:

$$\begin{aligned}
 & \frac{1}{d} \left(\left(\kappa_{i+1/2,j} \frac{(T_{i+1,j} - T_{i,j})}{d} - \kappa_{i-1/2,j} \frac{(T_{i,j} - T_{i-1,j})}{d} \right) + \right. \\
 & \quad \left. \left(\kappa_{i,j+1/2} \frac{(T_{i,j+1} - T_{i,j})}{d} - \kappa_{i,j-1/2} \frac{(T_{i,j} - T_{i,j-1})}{d} \right) \right) \\
 (3.26) \qquad \qquad \qquad & = f_{ij}(x, y, t).
 \end{aligned}$$

to get an truncation error at $O(d^2)$. Thus coefficients. γ_k are:

$$\begin{aligned}
 \gamma_1 &= \frac{\kappa_{i-1/2,j}}{d^2}, & \gamma_2 &= -\frac{1}{d^2}(\kappa_{i+1/2,j} + \kappa_{i-1/2,j} + \kappa_{i,j+1/2} + \kappa_{i,j-1/2}) \\
 \gamma_3 &= \frac{\kappa_{i+1/2,j}}{d^2}, & \gamma_4 &= \frac{\kappa_{i,j-1/2}}{d^2} & \gamma_5 &= \frac{\kappa_{i,j+1/2}}{d^2}. & \gamma_6 &= 0.
 \end{aligned}$$

with

$$C_{ij} = 0$$

Figure 3.2: The geometry at an irregular grid point (i, j)

2. At an *irregular point*, we still want to determine the coefficients γ_i 's in the form (3.25). Since these points are adjacent to the curve Γ and form a lower-dimension set, it is enough to require an $O(h)$ truncation error at these points. We could follow the same procedure as in one dimension and expand all the $T_{i+i_k, j+j_k}$ about some point (x_i^*, y_j^*) on the interface Γ . In one dimension, there is only one such point α . But in two dimensions we can choose more than one point (x_i^*, y_j^*) . For example, we could choose (x_i^*, y_j^*) as the point closest to (x_i, y_j) as shown

in the Figure (3.2). We can expand each $T_{i+i_k, j+j_k}$ about (x^*, y^*) . Here we use the superscripts $-$ or $+$ to denote the limiting values of a function from one side or the other. As an example, in the configuration shown in Fig. (3.2), we would expand

$$\begin{aligned}
 T(x_i, y_j) &= T^- + T_x^-(x_i - x_i^*) + T_y^-(y_j - y_j^*) + \frac{1}{2}T_{xx}^-(x_i - x_i^*)^2 \\
 (3.27) \quad &+ \frac{1}{2}T_{yy}^-(y_j - y_j^*)^2 + T_{xy}^-(x_i - x_i^*)(y_j - y_j^*) + O(h^3).
 \end{aligned}$$

$$\begin{aligned}
 T(x_{i+1}, y_j) &= T^+ + T_x^+(x_{i+1} - x_i^*) + T_y^+(y_j - y_j^*) + \frac{1}{2}T_{xx}^+(x_{i+1} - x_i^*)^2 \\
 (3.28) \quad &+ \frac{1}{2}T_{yy}^+(y_j - y_j^*)^2 + T_{xy}^+(x_{i+1} - x_i^*)(y_j - y_j^*) + O(h^3).
 \end{aligned}$$

If we do this expansion at each point used in the difference equation (3.24), then the local truncation error T_{ij} can be expressed as a linear combination of the values $T^\pm, T_x^\pm, T_y^\pm, T_{xx}^\pm, T_{xy}^\pm, T_{yy}^\pm$. Following the one-dimensional derivation, we wish to eliminate all values on one side of the interface $T^+, T_x^+, T_y^+, T_{xx}^+, T_{xy}^+, T_{yy}^+$ in terms of the values on the other side, $T^-, T_x^-, T_y^-, T_{xx}^-, T_{xy}^-, T_{yy}^-$. Here the jump conditions will be used.

$$(3.29) \quad [T] = T^+ - T^- = \frac{q}{h}.$$

$$(3.30) \quad \kappa^- \frac{\partial T^-}{\partial n} = \kappa^+ \frac{\partial T^+}{\partial n}.$$

where $\frac{\partial}{\partial n}$ represents differentiation in a direction normal to the interface. From (3.29) we get the information in the tangential direction, while (3.30) gives information in the normal direction. In order to manipulate the above equations and perform the desired elimination, it turns out to be convenient to transfer from global coordinates into local coordinates with directions ξ , normal to Γ and η , tangential to Γ .

Once T_{ij} is expressed as a linear combination of the values $T^-, T_x^-, T_{xx}^-, T_y^-, T_{xy}^-, T_{yy}^-$, let all the coefficients of each of these terms vanishes to ensure the $O(h)$ truncation error. This leads to a linear system of six equations that determine the coefficients γ_k . So instead of a five-point stencil, we need an extra point to uniquely determine the coefficients.

To determine the difference scheme at an irregular grid point we

take the following steps.

- Select a point $(x_i^*, y_j^*) \in \Gamma$ near (x_i, y_j) . Here we choose the projection of the point (x_i, y_j) onto the interface.
- Apply a local coordinate transformation in directions normal and tangential to Γ at the point (x_i^*, y_j^*) . We assume that the equation for Γ is given as data.
- Derive relations between each side in the local coordinates.
- Choose an additional point to form a six-point stencil.
- Establish and solve a linear system of six equations to determine the coefficients γ_k .

Transformation to Local Coordinates

First we have to choose a point (x_i^*, y_j^*) on the interface. We usually take this point as the projection of (x_i, y_j) onto the interface when the interface is smooth at this point. Otherwise we could take any smooth point on the interface in the neighborhood of (x_i, y_j) , possibly the nearest point.

Based on the point (x_i^*, y_j^*) , we apply a local coordinate transformation. Generally, the transformation is equal to translation followed by a rotation. Let θ be the angle between the x-axis and the outside normal direction of the interface ξ , pointing in the positive direction. The transformation is²:

$$\begin{bmatrix} \xi \\ \eta \end{bmatrix} = \begin{bmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{bmatrix} \begin{bmatrix} x - x_i^* \\ y - y_j^* \end{bmatrix}$$

so :

$$\begin{aligned} \xi &= (x - x_i^*) \cos \theta + (y - y_j^*) \sin \theta \\ (3.31) \quad \eta &= -(x - x_i^*) \sin \theta + (y - y_j^*) \cos \theta \quad . \end{aligned}$$

²we call

$$\begin{bmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{bmatrix}$$

a 2D rotation matrix

The interface relations in the local coordinates for two-dimensional problems

We consider a fixed point (x_i^*, y_j^*) and define a new $\xi - \eta$ coordinate system based on the directions normal and tangential to Γ at this point using (3.31). In the neighborhood of this point, the interface lies roughly in the η -direction, so we can parameterize Γ locally by $\xi = \chi(\eta), \eta = \eta$. Since $\chi(0) = 0$ and, provided the boundary is smooth at (x_i^*, y_j^*) , $\chi'(0) = 0$ as well. The details are shown in the appendix.

In the local coordinates, we can write equation (3.29) as:

$$(3.32) \quad T^+(\chi(\eta), \eta) - T^-(\chi(\eta), \eta) = \frac{q_n}{h} = \omega(\eta).$$

In this case q_n is the heat flux normal to the embedded boundary. It is continuous along the interface. So, differentiating this with respect to η along the interface, gives

$$(3.33) \quad [T_\xi]\chi' + [T_\eta] = \omega'(\eta)$$

where $[T_\xi] = T_\xi^+ - T_\xi^-$ and $[T_\eta] = T_\eta^+ - T_\eta^-$.

Differentiating again with respect to η gives:

$$(3.34) \quad [T_{\xi\xi}]\chi'^2 + 2[T_{\xi\eta}]\chi' + [T_\xi]\chi'' + [T_{\eta\eta}] = \omega''(\eta).$$

at $\eta = 0$, $\chi'(0) = 0$, and we get the two jump conditions:

$$(3.35) \quad T^+(\chi(\eta), \eta) - T^-(\chi(\eta), \eta) = \frac{q_n}{h} = \omega(\eta).$$

$$(3.36) \quad [T_{\xi\xi}]\chi'' + [T_{\eta\eta}] = \omega''(0).$$

Also we have jump condition (3.30) on Γ . At a point $(\chi(\eta), \eta) \in \Gamma$, from the mathematical derivation, we could obtain the normal derivative in terms of ξ and η derivatives as:

$$\frac{\partial T}{\partial n} = \frac{1}{\sqrt{1 + \chi'^2}}(T_\xi - T_\eta \chi').$$

so the equation (3.30) becomes

$$(3.37) \quad \kappa^+(T_\xi^+ - T_\eta^+ \chi') = \kappa^-(T_\xi^- - T_\eta^- \chi').$$

Differentiating this with respect to η gives:

$$(3.38) \quad [\kappa(T_{\xi\xi}\chi' + T_{\xi\eta} - T_\eta\chi'' - T_{\xi\eta}\chi'^2 - T_{\eta\eta}\chi')] = 0.$$

Evaluating (3.37) and (3.38) at $\eta = 0$ gives more jump conditions:

$$(3.39) \quad [\kappa T_\xi] = 0.$$

$$(3.40) \quad [\kappa(T_{\xi\eta} - T_{\eta}\chi'')] = 0.$$

We can use the relations (3.37) - (3.40) to eliminate the values on the + side of Γ in terms of values on the - side. setting:

$$\rho = \frac{\kappa^-}{\kappa^+}.$$

the jump relations are given by:(at $\xi = \eta = 0$)

$$T^+ = T^- + \omega(0)$$

$$T_{\xi}^+ = \rho T_{\xi}^-$$

$$T_{\eta}^+ = T_{\eta}^- + \omega'(0)$$

$$T_{\eta\eta}^+ = T_{\eta\eta}^- + (T_{\xi}^- - T_{\xi}^+)\chi'' + \omega''(0)$$

$$(3.41) \quad T_{\xi\eta}^+ = \rho T_{\xi\eta}^- + (1 - \rho)T_{\eta}^-\chi''$$

From the PDE (3.24), we get:

$$(3.42) \quad \begin{aligned} \kappa^+ T_{\xi\xi}^+ + \kappa^+ T_{\eta\eta}^+ + \kappa_{\xi}^+ + \kappa_{\eta}^+ &= \kappa^- T_{\xi\xi}^- + \kappa^- T_{\eta\eta}^- + \kappa_{\xi}^- + \kappa_{\eta}^- \\ T_{\xi\xi}^+ &= \frac{\kappa^-}{\kappa^+} T_{\xi\xi}^- + \frac{\kappa_{\xi}^-}{\kappa^+} T_{\eta\eta}^- - T_{\eta\eta}^+ \\ &+ \frac{\kappa_{\xi}^-}{\kappa^+} T_{\xi}^- - \frac{\kappa_{\xi}^+}{\kappa^+} T_{\xi}^+ + \frac{\kappa_{\eta}^-}{\kappa^+} T_{\eta}^- - \frac{\kappa_{\eta}^+}{\kappa^+} T_{\eta}^+ + \frac{[f]}{\kappa^+}. \end{aligned}$$

Because $\kappa_\xi = \kappa_\eta = 0$, we can simplify the above equation as:

$$(3.43) \quad T_{\xi\xi}^+ = \rho T_{\xi\xi}^- + (\rho - 1)T_{\eta\eta}^- - (\rho - 1)T_\xi^- \chi'' - \omega''(0)$$

The derivation of the difference method for irregular points

Now, we are ready to derive the difference scheme for an irregular point. First, let us denote the $\xi - \eta$ coordinates of the six points in the difference stencil (as we mentioned at beginning of this section)

$$(x_{i-1}, y_j), (x_i, y_j), (x_{i+1}, y_j), (x_i, y_{j-1}), (x_i, y_{j+1}), (x_{i+i_0}, y_{j+j_0}).$$

as

$$(\xi_1, \eta_1), (\xi_2, \eta_2), (\xi_3, \eta_3), (\xi_4, \eta_4), (\xi_5, \eta_5), (\xi_6, \eta_6)$$

Respectively, then the local truncation error T_{ij} of the difference scheme at (x_i, y_j) becomes:

$$(3.44) \quad \begin{aligned} T_{ij} = & \gamma_1 T(\xi_1, \eta_1) + \gamma_2 T(\xi_2, \eta_2) + \gamma_3 T(\xi_3, \eta_3) + \gamma_4 T(\xi_4, \eta_4) \\ & + \gamma_5 T(\xi_5, \eta_5) + \gamma_6 T(\xi_6, \eta_6) - f_{ij} - C_{ij}. \end{aligned}$$

Expand all the terms about (0,0) in local coordinates from each side of the interface. to obtain:

$$(3.45) \quad T(\xi_k, \eta_k) = T^\pm + \xi_k T_\xi^\pm + \eta_k T_\eta^\pm + \frac{1}{2} \xi_k^2 T_{\xi\xi}^\pm + \xi_k \eta_k T_{\xi\eta}^\pm + \frac{1}{2} \eta_k^2 T_{\eta\eta}^\pm + O(h^3).$$

where the choice of + and - sign is depends on whether (ξ_k, η) lies on the + or - side of Γ . Substituting (3.45) into (3.44) and collecting terms gives an expression of the form:

$$(3.46) \quad T_{ij} = a_1 T^- + a_2 T^+ + a_3 T_\xi^- + a_4 T_\xi^+ + a_5 T_\eta^- + a_6 T_\eta^+ + a_7 T_{\xi\xi}^- + a_8 T_{\xi\xi}^+ + a_9 T_{\eta\eta}^- + a_{10} T_{\eta\eta}^+ + a_{11} T_{\xi\eta}^- + a_{12} T_{\xi\eta}^+ - f_{ij} - C_{ij} + O(h).$$

where the a_j only depend on the position of the stencil relative to the interface and are given by:

$$\begin{aligned} a_1 &= \sum_{k \in \kappa^-} \gamma_k & a_2 &= \sum_{k \in \kappa^+} \gamma_k \\ a_3 &= \sum_{k \in \kappa^-} \xi_k \gamma_k & a_4 &= \sum_{k \in \kappa^+} \xi_k \gamma_k \end{aligned}$$

$$\begin{aligned}
a_5 &= \sum_{k \in \kappa^-} \eta_k \gamma_k & a_6 &= \sum_{k \in \kappa^+} \eta_k \gamma_k \\
a_7 &= \frac{1}{2} \sum_{k \in \kappa^-} \xi_k^2 \gamma_k & a_8 &= \frac{1}{2} \sum_{k \in \kappa^+} \xi_k^2 \gamma_k \\
a_9 &= \frac{1}{2} \sum_{k \in \kappa^-} \eta_k^2 \gamma_k & a_{10} &= \frac{1}{2} \sum_{k \in \kappa^+} \eta_k^2 \gamma_k \\
a_{11} &= \sum_{k \in \kappa^-} \xi_k \eta_k \gamma_k & a_{12} &= \sum_{k \in \kappa^+} \xi_k \eta_k \gamma_k
\end{aligned}
\tag{3.47}$$

Combining (3.41), (3.43), (3.46) and rearranging, we obtain:

$$\begin{aligned}
T_{ij} &= (a_1 + a_2)T^- + (a_3 + \rho a_4 - a_8(1 - \rho)\chi'' + a_{10}(1 - \rho)\chi'')T_\xi^- \\
&\quad + (a_5 + a_6 + a_{12}(1 - \rho)\chi'')T_\eta^- + (a_7 + a_8(\frac{\kappa_-}{\kappa_+}))T_{\xi\xi}^- \\
&\quad + (a_8(\frac{\kappa_-}{\kappa_+}) - a_8 + a_9 + a_{10})T_{\eta\eta}^- + (a_{11} + \rho a_{12})T_{\xi\eta}^- \\
&\quad \hat{T}_{ij} - f_{ij} - C_{ij} + O(h)
\end{aligned}
\tag{3.48}$$

and $\hat{T}_{ij} = a_2\omega(\eta) + a_6\omega'(\eta) + a_8\omega''(\eta) + a_{10}\omega''(\eta)$

where $\omega(\eta) = \frac{\kappa^- T_\xi^-}{h} = \frac{\kappa^+ T_\xi^+}{h} = \frac{q_n}{h}$

Since the flux is continuous in the whole domain, it can be treated as constant when the boundary condition is fixed, and $\omega'(\eta) = 0, \omega''(\eta) = 0$. so

$$\hat{T}_{ij} = a_2\omega(\eta)$$

Here, we still use the relation of PDE on the left side (3.24)

$$\kappa^-(T_{\eta\eta}^- + T_{\xi\xi}^-) + \kappa_\xi^- T_\xi^- + \kappa_\eta^- T_\eta^- - f_{ij}^- = 0$$

We can ensure $T_{ij} = O(h)$ by making each coefficient of T^- , T_ξ^- , T_η^- , $T_{\xi\xi}^-$, $T_{\xi\eta}^-$, and $T_{\eta\eta}^-$ vanish and $C_{ij} = 0$ as well. This will give six equations for the six unknowns $\gamma_1, \dots, \gamma_6$:

$$a_1 + a_2 = 0$$

$$a_3 + \rho a_4 - (1 - \rho)(a_{10} - a_8)\chi'' - a_2\left(\frac{\kappa^-}{h}\right) = 0$$

$$a_5 + a_6 + a_{12}(1 - \rho)\chi'' = 0$$

$$a_7 + a_8\left(\frac{\kappa^-}{\kappa^+}\right) = -\kappa^-$$

$$a_8\left(\frac{\kappa^-}{\kappa^+}\right) - a_8 + a_9 + a_{10} = -\kappa^-$$

$$a_{11} + \rho a_{12} = 0$$

and

$$C_{ij} = 0.$$

These simultaneous equations can be solved for the coefficients γ 's. If $\kappa^- \kappa^+ > 0$, then the linear system has a unique solution. And even if $\kappa^- \kappa^+ < 0$, it

turns out only for some specific values of $[\kappa]$, the coefficients of matrix for the unknown γ_j 's are singular, so the algorithm is typically successful.

In order to solve the transient problem, we replace $f(x, t)$ by $C_p(\frac{\partial T}{\partial t})$. Discretizing in time with the explicit method, we obtain:

$$(3.49) \quad \begin{aligned} & \gamma_1 T_{i-1,j,t} + \gamma_2 T_{i,j,t} + \gamma_3 T_{i+1,j,t} + \gamma_4 T_{i,j-1,t} \\ & + \gamma_5 T_{i,j+1,t} + \gamma_6 T_{i+i_0,j+j_0,t} = C_p \frac{(T_{i,j,t+1} - T_{i,j,t})}{\Delta t} \end{aligned} .$$

or

$$T_{i,j,t+1} = \frac{\Delta t}{C_p} (\gamma_1 T_{i-1,j,t} + \gamma_2 T_{i,j,t} + \gamma_3 T_{i+1,j,t} + \gamma_4 T_{i,j-1,t} + \gamma_5 T_{i,j+1,t} + \gamma_6 T_{i+i_0,j+j_0,t}) + T_{i,j,t}.$$

3.3.2 Stability of the numerical solution in two dimensional problems

To ensure the stability of the explicit method or forward Euler numerical solution, we require the mesh sizes to satisfy the condition:

$$(3.50) \quad v_x + v_y \leq \frac{1}{2} \quad .$$

where

$$v_x = \frac{\alpha \Delta t}{(\Delta x)^2}, \quad v_y = \frac{\alpha \Delta t}{(\Delta y)^2}$$

$$\alpha = \frac{\kappa^\pm}{c_p}.$$

As in one dimension, we choose the smaller Δt for the two different κ .

3.4 Three-dimensional problem

Following the one-dimensional and two-dimensional problems, we now deal with the three-dimensional problems. In three dimensions, the form (3.6) becomes:

$$(3.51) \quad c_p \left(\frac{\partial T}{\partial t} \right) + (-\kappa T_x)_x + (-\kappa T_y)_y + (-\kappa T_z)_z = 0 \quad .$$

where κ is discontinuous across the interface.

The domain is chosen to be a cube. $[a, b] \times [a, b] \times [a, b]$. We take a uniform grid with:

$$x_i = a + id \quad y_j = a + jd \quad z_k = a + kd$$

$$i, j, k = 0, 1, 2, \dots, n$$

where

$$d = \frac{b - a}{n}$$

The same procedure will be followed as for the 2-D problem. but the interface in 3-D becomes is an surface instead of a curve in 2-D. Let us define the surface of the interface as Γ here and steps will be similar to those in 2-D problems:

1. Select a point $(x_i^*, y_j^*, z_k^*) \in \Gamma$ near (x_i, y_j, z_k) .
2. Apply a local coordinate transformation in three directions normal and tangential to Γ at (x_i^*, y_j^*, z_k^*) .

3. Derive the jump conditions relating $+$ and $-$ in the local coordinates.
4. Choose three additional points to form a ten-point stencil.
5. Establish and solve a linear system of ten equations for the coefficients γ_k .

3.4.1 Numerical solution in three-dimensional problems

The point (x_i^*, y_j^*, z_k^*) can be chosen arbitrarily, but most simply can be taken as the projection of point (x_i, y_j, z_k) onto the interface when it is smooth at that point, otherwise, it could be any other point on that interface, possibly the nearest point.

Transformation of coordinates

The transformation from global to local coordinates includes rotation and a translation. It can be expressed in the form:

$$\begin{bmatrix} \xi \\ \eta \\ \zeta \end{bmatrix} = R_{x\theta} R_{y\phi} R_{z\varphi} \begin{bmatrix} x - x_i^* \\ y - y_j^* \\ z - z_k^* \end{bmatrix}$$

where ξ, η are tangential directions, φ is the normal direction of the surface.

$R_{x\theta}, R_{y\phi}, R_{z\varphi}$ are rotation matrices:

$$R_{x\theta} = \begin{vmatrix} 1 & 0 & 0 \\ 0 & \cos \theta & \sin \theta \\ 0 & -\sin \theta & \cos \theta \end{vmatrix}$$

$$R_{y\phi} = \begin{vmatrix} \cos \phi & 0 & -\sin \phi \\ 0 & 1 & 0 \\ \sin \phi & 0 & \cos \phi \end{vmatrix}$$

$$R_{z\varphi} = \begin{vmatrix} \cos \varphi & \sin \varphi & 0 \\ -\sin \varphi & \cos \varphi & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

and θ is the angle between the x-axis and the normal direction of the surface (interface), ϕ is the angle between y-axis and normal direction of the surface and φ is the angle between the z-axis and the normal direction of the surface.

Derivation of the jump condition

Let us expand $T(x_i, y_j, z_k)$ about the point (x_i^*, y_j^*, z_k^*)

$$\begin{aligned}
 T(x_i, y_j, z_k) &= T^- + T_x^-(x_i - x_i^*) + T_y^-(y_j - y_j^*) + T_z^-(z_k - z_k^*) \\
 &+ T_{xy}^-(x_i - x_i^*)(y_j - y_j^*) + T_{yz}^-(y_j - y_j^*)(z_k - z_k^*) + T_{xz}^-(x_i - x_i^*)(z_k - z_k^*) \\
 &+ \frac{1}{2}T_{xx}^-(x_i - x_i^*)^2 + \frac{1}{2}T_{yy}^-(y_j - y_j^*)^2 + \frac{1}{2}T_{zz}^-(z_k - z_k^*)^2.
 \end{aligned}
 \tag{3.52}$$

$$\begin{aligned}
 T(x_{i+1}, y_j, z_k) &= T^+ + T_x^+(x_{i+1} - x_i^*) + T_y^+(y_j - y_j^*) + T_z^+(z_k - z_k^*) \\
 &+ T_{xy}^+(x_{i+1} - x_i^*)(y_j - y_j^*) + T_{yz}^+(y_j - y_j^*)(z_k - z_k^*) + T_{xz}^+(x_{i+1} - x_i^*)(z_k - z_k^*) \\
 &+ \frac{1}{2}T_{xx}^+(x_{i+1} - x_i^*)^2 + \frac{1}{2}T_{yy}^+(y_j - y_j^*)^2 + \frac{1}{2}T_{zz}^+(z_k - z_k^*)^2.
 \end{aligned}
 \tag{3.53}$$

The jump condition in 3D is :

$$[T] = T^+ - T^- = \frac{q\zeta}{h} = \omega(\xi, \eta).
 \tag{3.54}$$

$$(3.55) \quad \kappa^+ T_\zeta^+ = \kappa^- T_\zeta^- = \kappa^\pm \frac{\partial T}{\partial \zeta}.$$

where q_ζ is the heat flux along the normal direction of the surface, which is continuous along the interface. $\zeta = \chi(\xi, \eta)$ is the parametric representation of the interface in the neighborhood of the point (ξ, η, ζ) .

Our goal is again to develop a finite difference equation of the form

$$(3.56) \quad \sum_k \gamma_m T_{i+i_m, j+j_m, k+k_m} = -f(t).$$

As in the one dimensional and two dimensional problems, we have two different cases of regular and irregular points.

1. Regular points are the points for which there is no interface located between the seven points in the stencil. At these points, $O(h^2)$ truncation is achieved by using the standard seven-point stencil

$$\begin{aligned} & \frac{1}{d} \left(\left(\kappa_{i+1/2, j, k} \frac{(T_{i+1, j, k} - T_{i, j, k})}{d} - \kappa_{i-1/2, j, k} \frac{(T_{i+1, j, k} - T_{i, j, k})}{d} \right) \right. \\ & \left. + \left(\kappa_{i, j+1/2, k} \frac{(T_{i, j+1, k} - T_{i, j, k})}{d} - \kappa_{i, j-1/2, k} \frac{(T_{i, j, k} - T_{i, j-1, k})}{d} \right) \right) \end{aligned}$$

$$(3.57) \quad \left(\kappa_{i,j,k+1/2} \frac{(T_{i,j,k+1} - T_{i,j,k})}{d} - \kappa_{i,j,k-1/2} \frac{(T_{i,j,k} - T_{i,j,k-1})}{d} \right).$$

Corresponding to equation (3.56), we obtain:

$$\gamma_1 = \frac{\kappa_{i-1/2,j,k}}{d^2}$$

$$\gamma_2 = -\frac{1}{d^2}(\kappa_{i+1/2,j,k} + \kappa_{i-1/2,j,k} + \kappa_{i,j+1/2,k} + \kappa_{i,j-1/2,k} + \kappa_{i,j,k+1/2} + \kappa_{i,j,k-1/2})$$

$$\gamma_3 = \frac{1}{d^2}(\kappa_{i+1/2,j,k}) \quad \gamma_4 = \frac{1}{d^2}(\kappa_{i,j-1/2,k})$$

$$\gamma_5 = \frac{1}{d^2}(\kappa_{i,j+1/2,k}) \quad \gamma_6 = \frac{1}{d^2}(\kappa_{i,j,k-1/2})$$

$$\gamma_7 = \frac{1}{d^2}(\kappa_{i,j,k+1/2}) \quad \gamma_8 = \gamma_9 = \gamma_{10} = 0.$$

2. For irregular points, an interface $\zeta = \chi(\eta, \xi)$ exists between some points in the seven-point stencil. Differentiating equation (3.54) with respect to ξ, η gives:

$$(3.58) \quad [T_\zeta]\chi_\xi + [T_\xi] = \omega_\xi(\xi, \eta).$$

$$(3.59) \quad [T_\zeta]\chi_\eta + [T_\eta] = \omega_\eta(\xi, \eta).$$

Differentiating again with respect to ξ, η gives:

$$(3.60) \quad [T_{\zeta\zeta}]\chi_\xi^2 + 2[T_{\zeta\xi}]\chi_\xi + [T_\zeta]\chi_{\xi\xi} + [T_{\xi\xi}] = \omega_{\xi\xi}(\xi, \eta).$$

$$(3.61) \quad [T_{\zeta\zeta}]\chi_\eta^2 + 2[T_{\zeta\eta}]\chi_\eta + [T_{\zeta}]\chi_{\eta\eta} + [T_{\eta\eta}] = \omega_{\eta\eta}(\xi, \eta).$$

$$(3.62) \quad [T_{\zeta}]\chi_{\xi\xi} + [T_{\xi\xi}] = \omega_{\xi\xi}(\xi, \eta).$$

$$(3.63) \quad [T_{\zeta}]\chi_{\eta\eta} + [T_{\eta\eta}] = \omega_{\eta\eta}(\xi, \eta).$$

Expressing the normal derivative in terms of (ξ, η, ζ)

$$(3.64) \quad \frac{\partial T}{\partial \zeta} = \frac{1}{\sqrt{1 + \chi_\xi^2 + \chi_\eta^2}}(T_\zeta - T_\xi \chi_\xi - T_\eta \chi_\eta).$$

The jump condition

$$\kappa^- \left(\frac{\partial T}{\partial \zeta} \right)^- = \kappa^+ \left(\frac{\partial T}{\partial \zeta} \right)^+.$$

becomes:

$$(3.65) \quad \kappa^- \frac{1}{\sqrt{1 + \chi_\xi^2 + \chi_\eta^2}}(T_\zeta^- - T_\xi^- \chi_\xi - T_\eta^- \chi_\eta) = \kappa^+ \frac{1}{\sqrt{1 + \chi_\xi^2 + \chi_\eta^2}}(T_\zeta^+ - T_\xi^+ \chi_\xi - T_\eta^+ \chi_\eta).$$

so:

$$(3.66) \quad \kappa^- (T_\zeta^- - T_\xi^- \chi_\xi - T_\eta^- \chi_\eta) = \kappa^+ (T_\zeta^+ - T_\xi^+ \chi_\xi - T_\eta^+ \chi_\eta).$$

Differentiating this with respect to ξ or η gives more jump conditions

at $\xi = \eta = 0$ and $\chi_\xi = \chi_\eta = 0$:

$$(3.67) \quad [\kappa T_\zeta] = 0.$$

$$(3.68) \quad [\kappa(T_{\zeta,\xi} - T_\xi \chi_{\xi\xi} - T_\eta \chi_{\xi\eta})] = 0.$$

$$(3.69) \quad [\kappa(T_{\zeta\eta} - T_\eta \chi_{\eta\eta} - T_\xi \chi_{\xi\eta})] = 0.$$

We can use the relations above to derive more as follows. Setting:

$$\rho = \frac{\kappa^-}{\kappa^+}.$$

We could express the values on the $+$ side in terms of the $-$ side using the relations from (3.54) to (3.69).

$$(3.70) \quad T^+ - T^- = \omega(0, 0).$$

$$(3.71) \quad T_\zeta^+ = \rho T_\zeta^-.$$

$$(3.72) \quad T_\xi^+ = T_\xi^- + \omega_\xi(0, 0).$$

$$(3.73) \quad T_\eta^+ = T_\eta^- + \omega_\eta(0, 0).$$

$$(3.74) \quad T_{\xi\xi}^+ = T_{\xi\xi}^- + (T_\zeta^- - T_\zeta^+) \chi_{\xi\xi} + \omega_{\xi\xi}(0, 0).$$

$$(3.75) \quad T_{\eta\eta}^+ = T_{\eta\eta}^- + (T_\zeta^- - T_\zeta^+) \chi_{\eta\eta} + \omega_{\eta\eta}(0, 0).$$

$$(3.76) \quad T_{\zeta,\xi}^+ = \rho T_{\zeta\xi}^- + T_\xi^+ \chi_{\xi\xi} - \rho T_\xi^- \chi_{\xi\xi} - \rho T_\eta^- \chi_{\xi\eta} + T_\eta^+ \chi_{\xi\eta}.$$

$$(3.77) \quad T_{\zeta,\eta}^+ = \rho T_{\zeta\eta}^- + T_{\eta}^+ \chi_{\eta\eta} - \rho T_{\eta}^- \chi_{\eta\eta} - \rho T_{\xi}^- \chi_{\xi\eta} + T_{\xi}^+ \chi_{\xi\eta}.$$

We can differentiate $T_{\xi}^+ = T_{\xi}^- + \omega_{\xi}(\xi, \eta)$ with respect to η at $\xi = \eta = 0$ and get:

$$(3.78) \quad T_{\xi\eta}^+ = T_{\xi\eta}^- + \omega_{\xi\eta}(0, 0).$$

From the 3D governing PDE (3.51), we obtain:

$$(3.79) \quad \begin{aligned} T_{\zeta\zeta}^+ &= \frac{\kappa_{\zeta}^-}{\kappa^+} T_{\zeta\zeta}^- + \frac{\kappa_{\xi}^-}{\kappa^+} T_{\xi\xi}^- + \frac{\kappa_{\eta}^-}{\kappa^+} T_{\eta\eta}^- + \frac{\kappa_{\zeta}^- T_{\zeta}^-}{\kappa^+} + \frac{\kappa_{\eta}^- T_{\eta}^-}{\kappa^+} + \frac{\kappa_{\xi}^- T_{\xi}^-}{\kappa^+} \\ &\quad - T_{\eta\eta}^+ - T_{\xi\xi}^+ - \left(\frac{\kappa_{\xi}^+}{\kappa^+} T_{\xi}^+ + \frac{\kappa_{\eta}^+}{\kappa^+} T_{\eta}^+ + \frac{\kappa_{\zeta}^+}{\kappa^+} T_{\zeta}^+ \right) + \frac{[f]}{\kappa^+}. \end{aligned}$$

With the assumption that $\kappa_{\xi} = \kappa_{\eta} = \kappa_{\zeta} = 0$ and $[f] = 0$. (3.79)

becomes:

$$(3.80) \quad \begin{aligned} T_{\zeta\zeta}^+ &= \rho T_{\zeta\zeta}^- + (\rho - 1) T_{\xi\xi}^- + (\rho - 1) T_{\eta\eta}^- + (\rho - 1) T_{\zeta}^- (T_{\zeta\zeta}^- + T_{\xi\xi}^-) \\ &\quad - (\omega_{\xi\xi}(0, 0) + \omega_{\eta\eta}(0, 0)). \end{aligned}$$

The derivation of the difference scheme for irregular points in three dimension problem

- First, denote the ξ, η, ζ coordinates of the ten points in the difference stencil:

$$\begin{aligned}
& (x_{i-1}, y_j, z_k) \quad (x_i, y_j, z_k) \quad (x_{i+1}, y_j, z_k) \\
& (x_i, y_{j-1}, z_k) \quad (x_i, y_{j+1}, z_k) \quad (x_i, y_j, z_{k-1}) \\
& (x_i, y_j, z_{k+1}) \quad (x_{i+i_0}, y_{j+j_0}, z_k) \quad (x_{i+i_0}, y_j, z_{k+k_0}) \quad (x_i, y_{j+j_0}, z_{k+k_0})
\end{aligned}$$

as:

$$\begin{aligned}
& (\xi_1, \eta_1, \zeta_1), \quad (\xi_2, \eta_2, \zeta_2), \quad (\xi_3, \eta_3, \zeta_3) \\
& (\xi_4, \eta_4, \zeta_4), \quad (\xi_5, \eta_5, \zeta_5), \quad (\xi_6, \eta_6, \zeta_6) \\
& (\xi_7, \eta_7, \zeta_7), \quad (\xi_8, \eta_8, \zeta_8), \quad (\xi_9, \eta_9, \zeta_9) \quad (\xi_{10}, \eta_{10}, \zeta_{10})
\end{aligned}$$

- Now, we express the local truncation error (3.56) at the point (x_i, y_j, z_k) in local coordinates as:

$$\begin{aligned}
t_{i,j,k} = & \gamma_1 T(\xi_1, \eta_1, \zeta_1) + \gamma_2 T(\xi_2, \eta_2, \zeta_2) + \gamma_3 T(\xi_3, \eta_3, \zeta_3) + \gamma_4 T(\xi_4, \eta_4, \zeta_4) + \\
& \gamma_5 T(\xi_5, \eta_5, \zeta_5) + \gamma_6 T(\xi_6, \eta_6, \zeta_6) + \gamma_7 T(\xi_7, \eta_7, \zeta_7) + \gamma_8 T(\xi_8, \eta_8, \zeta_8) \\
(3.81) \quad & + \gamma_9 T(\xi_9, \eta_9, \zeta_9) + \gamma_{10} T(\xi_{10}, \eta_{10}, \zeta_{10}).
\end{aligned}$$

Expanding all the terms about $(0,0,0)$ in the local coordinates from

each side of the interface Γ , we get:

$$\begin{aligned}
(3.82) \quad T(\xi, \eta, \zeta) &= T^\pm + \xi_k T_\xi^\pm + \eta_k T_\eta^\pm + \zeta_k T_\zeta^\pm \\
&\quad + \frac{1}{2} \xi_k^2 T_{\xi\xi}^\pm + \frac{1}{2} \eta_k^2 T_{\eta\eta}^\pm + \frac{1}{2} \zeta_k^2 T_{\zeta\zeta}^\pm \\
&\quad + \xi_k \eta_k T_{\xi\eta}^\pm + \xi_k \zeta_k T_{\xi\zeta}^\pm + \eta_k \zeta_k T_{\eta\zeta}^\pm + O(d^3).
\end{aligned}$$

Substituting the above expansion into form (3.83) and collecting terms gives an expression of the form:

$$\begin{aligned}
(3.83) \quad t_{i,j,k} &= a_1 T^- + a_2 T^+ + a_3 T_\xi^- + a_4 T_\xi^+ + a_5 T_\eta^- \\
&\quad + a_6 T_\eta^+ + a_7 T_\zeta^- + a_8 T_\zeta^+ + a_9 T_{\xi\xi}^- + a_{10} T_{\xi\xi}^+ \\
&\quad + a_{11} T_{\eta\eta}^- + a_{12} T_{\eta\eta}^+ + a_{13} T_{\zeta\zeta}^- + a_{14} T_{\zeta\zeta}^+ + a_{15} T_{\xi\eta}^- + a_{16} T_{\xi\eta}^+ \\
&\quad + a_{17} T_{\xi\zeta}^- + a_{18} T_{\xi\zeta}^+ + a_{19} T_{\eta\zeta}^- + a_{20} T_{\eta\zeta}^+ - f_{i,j,k} - C_{i,j} + O(d).
\end{aligned}$$

then the a_j are defined by:

$$a_1 = \sum_{k \in \kappa^-} \gamma_k \quad a_2 = \sum_{k \in \kappa^+} \gamma_k$$

$$a_3 = \sum_{k\epsilon\kappa^-} \xi_k \gamma_k \quad a_4 = \sum_{k\epsilon\kappa^+} \xi_k \gamma_k$$

$$a_5 = \sum_{k\epsilon\kappa^-} \eta_k \gamma_k \quad a_6 = \sum_{k\epsilon\kappa^+} \eta_k \gamma_k$$

$$a_7 = \sum_{k\epsilon\kappa^-} \zeta_k \gamma_k \quad a_8 = \sum_{k\epsilon\kappa^+} \zeta_k \gamma_k$$

$$a_9 = \sum_{k\epsilon\kappa^-} \frac{1}{2} \xi_k^2 \gamma_k \quad a_{10} = \sum_{k\epsilon\kappa^+} \frac{1}{2} \xi_k^2 \gamma_k$$

$$a_{11} = \sum_{k\epsilon\kappa^-} \frac{1}{2} \eta_k^2 \gamma_k \quad a_{12} = \sum_{k\epsilon\kappa^+} \frac{1}{2} \eta_k^2 \gamma_k$$

$$a_{13} = \sum_{k\epsilon\kappa^-} \frac{1}{2} \zeta_k^2 \gamma_k \quad a_{14} = \sum_{k\epsilon\kappa^+} \frac{1}{2} \zeta_k^2 \gamma_k$$

$$a_{15} = \sum_{k \in \kappa^-} \xi_k \eta_k \gamma_k \quad a_{16} = \sum_{k \in \kappa^+} \xi_k \eta_k \gamma_k$$

$$a_{17} = \sum_{k \in \kappa^-} \xi_k \zeta_k \gamma_k \quad a_{18} = \sum_{k \in \kappa^+} \xi_k \zeta_k \gamma_k$$

$$a_{19} = \sum_{k \in \kappa^-} \eta_k \zeta_k \gamma_k \quad a_{20} = \sum_{k \in \kappa^+} \eta_k \zeta_k \gamma_k$$

Use the jump relations (3.54) to express all the terms in – (3.83)

becomes:

$$\begin{aligned} t_{i,j,k} = & a_1 T^- + a_2 \left(T^- + \omega(\xi, \eta) \right) + a_3 T_\xi^- + a_4 \left(T_\xi^- + \omega_\xi(\xi, \eta) \right) + a_5 T_\eta^- \\ & + a_6 \left(T_\eta^- + \omega_\eta(\xi, \eta) \right) + a_7 T_\zeta^- + a_8 (\rho T_\zeta^-) \\ & + a_9 T_{\xi\xi}^- + a_{10} \left(T_{\xi\xi}^- + (T_\zeta^- - \rho T_\zeta^-) \chi_{\xi\xi} + \omega_{\xi\xi}(\xi, \eta) \right) \\ & + a_{11} T_{\eta\eta}^- + a_{12} \left(T_{\eta\eta}^- + (T_\zeta^- - \rho T_\zeta^-) \chi_{\eta\eta} + \omega_{\eta\eta}(\xi, \eta) \right) \end{aligned}$$

$$\begin{aligned}
& +a_{13}T_{\zeta\zeta}^- + a_{14}(\rho T_{\zeta\zeta}^- + (\rho - 1)T_{\xi\xi}^- + (\rho - 1)T_{\eta\eta}^- + \rho T_{\zeta}^-(\chi_{\xi\xi} + \chi_{\eta\eta})) \\
& - T_{\zeta}^-(\chi_{\xi\xi} + \chi_{\eta\eta}) - \omega_{\xi\xi}(\xi, \eta) - \omega_{\eta\eta}(\xi, \eta)) \\
& + a_{15}T_{\xi\eta} + a_{16}(T_{\xi\eta}^- + \omega_{\xi\eta}(\xi, \eta)) + a_{17}T_{\xi\zeta}^- \\
& + a_{18}(\rho T_{\xi\zeta}^- + (T_{\xi}^- + \omega_{\xi}(\xi, \eta))\chi_{\xi\xi} - \rho T_{\xi}^-\chi_{\xi\xi} - \rho T_{\eta}^-\chi_{\xi\eta} + \\
& (T_{\eta}^- + \omega_{\eta}(\xi, \eta))\chi_{\xi\eta}) + \\
& a_{19}T_{\eta\zeta}^- + a_{20}(\rho T_{\eta\zeta}^- + (T_{\eta}^- + \omega_{\eta}(\xi, \eta))\chi_{\eta\eta} + \rho T_{\eta}^-\chi_{\eta\eta} \\
& - \rho T_{\xi}^-\chi_{\xi\eta} + T_{\xi}^+\chi_{\xi\eta}) - f_{i,j,k} - C_{i,j,k} + O(d).
\end{aligned}
\tag{3.84}$$

Where:

$$\omega(\xi, \eta) = \frac{\kappa^- T_{\zeta}^-}{h} = \frac{\kappa^+ T_{\zeta}^+}{h} = \frac{q_{\zeta}}{h}.$$

Since the flux q is continuous on the radius direction in the domain, it will keep constant through the whole domain in the radius direction, and $\omega(\xi, \eta)$ becomes constant, so we could get:

$$\omega'_{\xi} = \omega'_{\eta} = 0.$$

$$\omega'_{\xi\xi} = \omega'_{\eta\eta} = \omega'_{\xi\eta} = \omega'_{\xi\zeta} = \omega'_{\eta\zeta} = 0.$$

At the point $\xi = 0, \eta = 0,$

$$\chi_\xi = \chi_\eta = \chi_\zeta = 0.$$

Here, we use the PDE (3.51) on the left side and obtain:

$$\begin{aligned} & \kappa_\xi^- T_\xi^- + \kappa^- T_{\xi\xi}^- + \kappa_\eta^- T_\eta + \kappa^- T_{\eta\eta}^- + \kappa_\zeta^- T_\zeta^- + \kappa^- T_{\zeta\zeta}^- + \\ (3.85) \quad & f_{i,j,k} = 0. \end{aligned}$$

Rearrange (3.84) and combining with (3.85), gives:

$$\begin{aligned} t_{i,j,k} = & T^-(a_1 + a_2) + T_\xi^-(a_3 + a_4 + a_{18}(1 - \rho)\chi_{\xi\xi} + a_{20}(1 - \rho)\chi_{\xi\eta}) \\ & + T_\eta^-(a_5 + a_6 + a_{18}(1 - \rho)\chi_{\xi\eta} + a_{20}(1 - \rho)\chi_{\eta\eta}) + \\ & T_\zeta^-(a_7 + \rho a_8 + a_{10}(1 - \rho)\chi_{\xi\xi} + a_{12}(1 - \rho)\chi_{\eta\eta} + a_{14}(\rho - 1)(\chi_{\xi\xi} + \chi_{\eta\eta})) \\ & + T_{\xi\xi}^-(a_9 + a_{10} + a_{14}(\rho - 1) + \kappa^-) + T_{\eta\eta}(a_{11} + a_{12} + a_{14}(\rho - 1) + \kappa^-) \end{aligned}$$

$$\begin{aligned}
& +T_{\zeta\zeta}^-(a_{13} + \rho a_{14} + \kappa^-) + T_{\xi\eta}(a_{15} + a_{16}) + T_{\xi\zeta}(a_{17} + \rho a_{18}) \\
(3.86) \quad & +T_{\eta\zeta}(a_{19} + \rho a_{20}) + a_2\omega(\xi, \eta) - C_{i,j,k} + O(d).
\end{aligned}$$

We need the coefficients of T^- , T_ξ^- , T_η^- , T_ζ^- , $T_{\xi\xi}^-$, $T_{\eta\eta}^-$, $T_{\zeta\zeta}^-$, $T_{\xi\eta}^-$, $T_{\eta\zeta}^-$, $T_{\xi\zeta}^-$ and $C_{i,j,k}$ to vanish in order to have the $t_{i,j,k} = O(d)$, so we have ten equations as follows:

$$\begin{aligned}
a_1 + a_2 &= 0 \\
a_3 + a_4 + a_{18}(1 - \rho)\chi_{\xi\xi} + a_{20}(1 - \rho)\chi_{\xi\eta} &= 0 \\
a_5 + a_6 + a_{18}(1 - \rho)\chi_{\xi\eta} + a_{20}(1 - \rho)\chi_{\eta\eta} &= 0 \\
a_7 + \rho a_8 + a_{10}(1 - \rho)\chi_{\xi\xi} + a_{12}(1 - \rho)\chi_{\eta\eta} + a_{14}(\rho - 1)(\chi_{\xi\xi} + \chi_{\eta\eta}) &= 0 \\
a_9 + a_{10} + a_{14}(\rho - 1) + \kappa^- &= 0 \\
a_{11} + a_{12} + a_{14}(\rho - 1) + \kappa^- &= 0 \\
a_{13} + \rho a_{14} + \kappa^- &= 0 \\
a_{15} + a_{16} &= 0 \\
a_{17} + \rho a_{18} &= 0 \\
(3.87) \quad a_{19} + \rho a_{20} &= 0.
\end{aligned}$$

and

$$C_{i,j,k} = a_2 \omega_{\xi,\eta}.$$

Solving these equations, we can get the solution of coefficients. γ 's.

Last, we put $f(t)$ back to $-c_p(\frac{\partial T}{\partial t})$ and obtain the form (3.56)

as:

$$\begin{aligned}
 & \gamma_1 T_{i-1,j,k} + \gamma_2 T_{i,j,k} + \gamma_3 T_{i+1,j,k} + \gamma_4 T_{i,j-1,k} + \gamma_5 T_{i,j+1,k} \\
 & + \gamma_6 T_{i,j,k-1} + \gamma_7 T_{i,j,k+1} + \gamma_8 T_{i+i_0,j+j_0,k} + \gamma_9 T_{i+i_0,j,k+k_0} \\
 (3.88) \quad & + \gamma_{10} T_{i,j+j_0,k+k_0} = c_p \left(\frac{\partial T}{\partial t} \right).
 \end{aligned}$$

where i_0, j_0, k_0 will take the value either -1 or $+1$.

Numerical stability in three dimension

The stability scheme of the explicit method for 3D problem can be stated as:

$$v_x + v_y + v_z \leq \frac{1}{2}.$$

where

$$v_x = \frac{\alpha \Delta t}{\Delta x^2} \quad v_y = \frac{\alpha \Delta t}{\Delta y^2} \quad v_z = \frac{\alpha \Delta t}{\Delta x^2}.$$

and

$$\alpha = \frac{\kappa^\pm}{c_p}.$$

We will take the smaller Δt value between the κ^- and κ^+ to ensure the numerical stability.

Chapter 4

Numerical results

Some numerical tests for one dimensional and two dimensional problems have been done to confirm the second order accuracy for LeVeque's immersed boundary method. Before going through all test cases in detail, let us consider how to deal with the different boundary conditions, i.e., Dirichlet, convection and flux boundary conditions.

In one dimension, the cases are very simple, and are not discussed here. This section describes how to handle these boundary conditions in 2D.

4.1 Boundary Conditions for LeVeque's Imbedded Boundary Method

Let us state some assumptions first and then give more detail for each separate case.

- All the nodes are contained within the physical boundary. i.e., in the interior of the domain.
- All nodes on the boundary are either C, D, PF or others¹, which we define the C is the node type of convective. D is the node type of Dirichlet and PF is the node type of prescribed flux.
- Except those nodes of type D, the vector of unknowns contains the temperatures at all nodes.

¹Here we assume that neighborhood of any node involved in a boundary condition will not also include an embedded boundary condition simultaneously.

4.1.1 Derivation of Coefficients for Convective Nodes in 2D

In 2D, a convective node may be missing 1, 2 or 3 neighbors of its five point stencil. Below is a derivation of entries in the vector of unknown temperatures and right hand side vector for each case.

1. Case 1. One missing member:

Figure 4.1: Case for one missing member of convection boundary condition

Let us define **G** to be a ghost node which represents a missing node, **GN** is a node in the stencil which lies in the same line as **G**. **R1**, **R2** denote the two remaining nodes. Nodes **GN**, **R1** and **R2** may be **PF**, **C**, **D** or others, all of which have entries in the vector of unknown temperature except **D**. Our goal is to use the convective constraint to

limit those ghost nodes.

As we know, the convective constraint is:

$$(4.1) \quad q = h(T_c - T_{Amb}).$$

where T_{Amb} is the ambient temperature. And we can discretize the constraint (4.1) in each direction that has a ghost node. A central difference ² is used to approximate q . It implies:

$$-\kappa \frac{\partial T}{\partial x} = h(T_c - T_{Amb}),$$

or

$$-\kappa \frac{(T_G - T_{GN})}{2dg} = h(T_c - T_{Amb}).$$

and

$$(4.2) \quad T_G = \frac{2h(dg)}{\kappa}(T_{Amb} - T_c) + T_{GN}.$$

- if G-GN lie in the x direction, $dg = x_G - x_C$ and $dr = dy$.
- if G-GN lie in the y direction, $dg = y_G - y_C$ and $dr = dx$.

²see reference [8] page .37

substitute T_G into the Laplacian. then:

$$\begin{aligned}\Delta^3 T_c &= \frac{T_{R1} - 2T_c + T_{R2}}{dr^2} + \frac{T_G - 2T_c + T_{GN}}{dg^2} \\ &= T_c \left(-2 \left(\frac{1}{dr^2} + \frac{1}{dg^2} + \frac{h}{\kappa(dg)} \right) \right) + T_{R2} \left(\frac{1}{dr^2} \right) \\ &\quad + T_{GN} \left(\frac{2}{dg^2} \right) + T_{R1} \left(\frac{1}{dr^2} \right) + T_{Amb} \left(\frac{2h}{\kappa(dg)} \right).\end{aligned}$$

2. Case 2: Two missing members

Figure 4.2: Case for two missing members of convection boundary condition

Here G1 and G2 denote the two resulting ghost nodes. Assume that they do not both lie in the same direction (we will leave this to three missing members case). As for the one member missing case. the convective constraint (4.1) for G1-GN1 implies:

$$-\kappa \frac{(T_{G1} - T_{GN1})}{2(dg1)} = h(T_c - T_{Amb}).$$

³ Δ represent second derivative $\frac{\partial^2}{\partial z^2}$

or

$$T_{G1} = \frac{2h(dg1)}{\kappa}(T_{Amb} - T_c) + T_{GN1}.$$

The convective constraint (4.1) for $G2 - GN2$ implies:

$$-\kappa \frac{(T_{G2} - T_{GN2})}{2(dg2)} = h(T_c - T_{Amb}).$$

or

$$T_{G2} = \frac{2h(dg2)}{\kappa}(T_{Amb} - T_c) + T_{GN2}.$$

- if G1-GN1 lie in the x direction, let $dg1 = x_{G1} - x_c$ and $dg2 = y_{G2} - y_c$.
- if G1-GN1 lie in the y direction, let $dg1 = y_{G1} - y_c$ and $dg2 = x_{G2} - x_c$.

Two ghost nodes, T_{G1} and T_{G2} , have been replaced by the other three unknown nodes in the domain T_c, T_{GN1}, T_{GN2} , we obtain Laplacian:

$$\begin{aligned} \Delta T_c &= \frac{T_{G1} - 2T_c + T_{GN1}}{(dg1)^2} + \frac{T_{G2} - 2T_c + T_{GN2}}{(dg2)^2} \\ &= T_c \left(-2 \left(\frac{1}{(dg1)^2} + \frac{1}{(dg2)^2} \right) - \frac{2h}{\kappa} \left(\frac{1}{(dg1)} + \frac{1}{(dg2)} \right) \right) \\ &\quad + T_{GN1} \left(\frac{2h}{\kappa(dg1)} \right) + T_{GN2} \left(\frac{2h}{\kappa(dg2)} \right) \\ &\quad + T_{Amb} \left(\frac{2h}{\kappa} \left(\frac{1}{(dg1)} + \frac{1}{(dg2)} \right) \right). \end{aligned}$$

3. Case 3: Three missing members:

Figure 4.3: Case for three missing member of convection boundary condition

There are three resulting ghost nodes in this case. Among them, there are two ghost nodes that must lie in the same direction. So the central difference can not be used in this direction. Let us denote the ghost nodes as G1, G2, and G3. GN2 will still be denoted as the node in the stencil which lies in the same line as G2. Now the convective constraint (4.1) will apply for G1, G2 and G3:

For G1:

$$-\kappa \frac{(T_{G1} - T_c)}{dg} = h(T_c - T_{Amb}),$$

or

$$T_{G1} = \frac{h(dg)}{\kappa}(T_{Amb} - T_c) + T_c.$$

For G3:

$$-\kappa \frac{(T_c - T_{G3})}{dg} = h(T_c - T_{Amb}),$$

or

$$T_{G3} = \frac{h(dg)}{\kappa}(T_c - T_{Amb}) + T_c.$$

For G2:

$$-\kappa \frac{(T_{G2} - T_{GN2})}{2(dg2)} = h(T_c - T_{Amb}),$$

or

$$T_{G2} = \frac{2h(dg2)}{\kappa}(T_{Amb} - T_c) + T_{GN2}.$$

- if G2-GN2 lies in the x direction. let $dg2 = x_{G2} - x_c$ and $dg = y_{G1} - y_c$.
- if G2-GN2 lies in the y direction, let $dg2 = y_{G2} - y_c$ and $dg2 = x_{G1} - x_c$.

Replaced all the ghost nodes by T_c and T_{GN2} , the Laplacian then is:

$$\begin{aligned} \Delta T_c &= \frac{T_{G1} - 2T_c + T_{G3}}{(dg)^2} + \frac{T_{G2} - 2T_c + T_{GN2}}{(dg2)^2} \\ &= T_c \left(\frac{-2}{(dg)^2} - \frac{h}{\kappa(dg2)} \right) + T_{GN2} \left(\frac{2}{(dg2)^2} \right) + T_{Amb} \left(\frac{h}{\kappa(dg2)} \right). \end{aligned}$$

4.1.2 Derivation of Coefficients for Prescribed Flux Nodes in 2D

In two dimensions (2D), a prescribed flux node may be missing 1, 2 or 3 neighbors of its 5 point stencil.

1. Case 1: One missing member:

Figure 4.4: Case for one missing member of flux boundary condition

This is treated the same as we defined in the Convection case. G is the resulting ghost node, GN denotes the node in the stencil which lies in the same line as G . $R1$ and $R2$ are two remaining nodes. They might be either PF , C , D or others, which PF is defined as the node types of prescribed flux, C is the node types of convective, D is the node types of Dirichlet. All those have entries in the vector of unknown temperatures except D . Any terms involving Dirichlet temperatures contribute to the

right-hand vector of unknowns.

The constraint $q = q_{prescribed}$ at PF implies:

$$-\kappa \frac{(T_G - T_{PF})}{dg} = q_{prescribed},$$

or

$$T_G = -\frac{(dg)q_{prescribed}}{\kappa} + T_{PF}.$$

where:

- if G-PF lies in the x direction, let $dg = x_G - x_{PF}$ and $dr = dy$.
- if G-PF lies in the y direction, let $dg = y_G - y_{PF}$ and $dr = dx$.

Then, the Laplacian becomes:

$$\begin{aligned} \Delta T_{PF} &= \frac{T_{R1} - 2T_{PF} + T_{R2}}{dr^2} + \frac{T_G - 2T_{PF} + T_{GN}}{dg^2} \\ &= T_{PF} \left(\left(\frac{-2}{dr^2} \right) + \left(\frac{-1}{dg^2} \right) \right) + T_{R2} \left(\frac{1}{dr^2} \right) + T_{GN} \left(\frac{1}{dg^2} \right) \\ &\quad + T_{R1} \left(\frac{1}{dr^2} \right) - \frac{q_{prescribed}}{\kappa(dg)}. \end{aligned}$$

2. Case 2. Two missing members:

Here, the two resulting ghost nodes are denoted G1 and G2.

Assume that they do not lie in the same direction (we will leave the

Figure 4.5: Case for two missing members of flux boundary condition

case of the three missing members). Now the constraint $q = q_{prescribed}$ will apply to both G1 and G2.

For G1: the constraint can be written as $q = q_{prescribed1}$ implies:

$$-\kappa \frac{(T_{G1} - T_{PF})}{dg1} = q_{prescribed1} ,$$

or

$$T_{G1} = -\frac{(dg1)q_{prescribed1}}{\kappa} + T_{PF} .$$

For G2: the constraint can be written as $q = q_{prescribed2}$ implies:

$$-\kappa \frac{(T_{G2} - T_{PF})}{dg2} = q_{prescribed2} ,$$

or

$$T_{G2} = -\frac{(dg2)q_{prescribed2}}{\kappa} + T_{PF}.$$

which

- if G1-GN1 lie in the x direction, let $dg1 = x_{G1} - x_{PF}$ and $dg2 = y_{G2} - y_{PF}$.
- if G1-GN1 lie in the y direction, let $dg1 = y_{G1} - y_{PF}$ and $dg2 = x_{G2} - x_{PF}$.

And Laplacian is :

$$\begin{aligned} \Delta T_{PF} &= \frac{T_{R1} - 2T_{PF} + T_{R2}}{dr^2} + \frac{T_G - 2T_{PF} + T_{GN}}{dg^2} \\ &= T_{PF} \left(-\frac{1}{(dg1)^2} - \frac{1}{(dg2)^2} \right) + T_{GN1} \left(\frac{1}{(dg1)^2} \right) + T_{GN2} \left(\frac{1}{(dg2)^2} \right) \\ &\quad - \frac{q_{prescribed1}}{\kappa(dg1)} - \frac{q_{prescribed2}}{\kappa(dg2)}. \end{aligned}$$

3. Case 3. Three missing members

In this case, just two nodes PF and GN2 are in the domain. so we need to apply the flux constraint three times to limit those ghost nodes G1, G2 and G3. For G1, using constraint $q = q_{prescribed1}$

Figure 4.6: Case for three missing member of flux boundary condition

$$-\kappa \frac{(T_{G1} - T_{PF})}{dg} = q_{prescribed1}.$$

or

$$T_{G1} = -\frac{(dg)q_{prescribed1}}{\kappa} + T_{PF}.$$

For G2, using constraint $q = q_{prescribed2}$

$$-\kappa \frac{(T_{G2} - T_{PF})}{dg2} = q_{prescribed2},$$

or

$$T_{G2} = -\frac{(dg2)q_{prescribed2}}{\kappa} + T_{PF}.$$

For G3, using constraint $q = q_{prescribed3}$

$$-\kappa \frac{(T_{G3} - T_{PF})}{dg} = q_{prescribed3},$$

or

$$T_{G3} = \frac{(dg)q_{prescribed3}}{\kappa} + T_{PF}.$$

which

- if G2-GN2 lies in the x direction, let $dg2 = x_{G2} - x_{PF}$ and $dg = y_{G1} - y_{PF}$.
- if G2-GN2 lies in the y direction, let $dg2 = y_{G2} - y_{PF}$ and $dg = x_{G1} - x_{PF}$.

Then the Laplacian is :

$$\begin{aligned} \Delta T_{PF} &= \frac{T_{R1} - 2T_{PF} + T_{R2}}{dr^2} + \frac{T_G - 2T_{PF} + T_{GN}}{dg^2} \\ &= T_{PF} \left(-\frac{1}{(dg2)^2} \right) + T_{GN2} \left(\frac{1}{(dg2)^2} \right) \\ &\quad - \frac{q_{prescribed1}}{\kappa(dg)} - \frac{q_{prescribed2}}{\kappa(dg2)} + \frac{q_{prescribed3}}{\kappa(dg)}. \end{aligned}$$

4.2 Computer Algorithm

In order to evaluate LeVeque's immersed interface method with discontinuous coefficients, computer programs were developed as a part of this

work. The first step is designed to solve steady state problems of the energy equation (3.6). The second step is designed to solve transient problems of equation (3.6) using explicit and implicit numerical methods.

Both programs require evaluation of the coefficients of the finite difference equation and the right hand side vector for the individual nodes and assembly of these coefficients and vectors to obtain the global stiffness matrices and vectors. The steady state problem of equation (3.6) involves a one solution of a set of simultaneous equations. The transient analysis program must solve such equations repeatedly to march in time.

To get the global coefficient matrices, we need to use the derivation from Chapter Three, of which two cases have been denoted.

1. For those nodes which are not involved in the embedded boundary, a standard five-point stencil in 2D is used in our method.
2. On the other hand, the nodes which are involved in the embedded boundary case, coefficients for the finite difference equation can not be obtained directly, so we need to solve three local equations in 1D and

six local equations in 2D⁴simultaneously to get the coefficients, just as shown in derivations in chapter three.

Also, the boundary conditions which have been derived in the last section need to be taken into account, because they also affect the coefficients of the equations. Here the assumption is: for every individual node, the boundary conditions and embedded boundary condition can not exist simultaneously. So, we need to make the domain large enough to avoid this happening.

In our main program, the following steps will be taken:

- Loop over each node in the domain which was defined.
- For each node, find which case it is (boundary, embedded boundary, or other).
- Calculate the coefficients of difference equation for each node according to its case.
- Solve the simultaneous equations using Meshach's⁵ solver which uses

⁴ten for the 3D, here we just test the cases for one dimension and two dimensions

⁵the person who design the software package for solving the matrix

an LDL^T factorization of the coefficient matrix. In a transient analysis, using the explicit method does not change the coefficient matrix over time steps, so the factorization of the matrix is not repeated in this case. But for the implicit method, we need to solve the global matrix for each node in each time step.

4.3 Case studies

Several tests for one dimension and for two dimensions have been set using the formulation which was developed in this work and outlined in Chapter 3. Also, the computer algorithms described in the earlier sections of this chapter are used in the computation. The results are presented later in this section.

4.3.1 Case study 1: *One dimensional test case*

In this study, a simple straight line has been selected for a one dimensional test as shown in figure (4.7). At point α , temperature is discontinuous, because of the contact conductance. Let us assume the materials on each side of the point α are different, so the thermal conductances are different.

Figure 4.7: Grids for the one dimension test case

The following data are used:

- **Geometry and Material Properties:**

Thermal Conductivity K_c = $40 \frac{J}{msK}$ (material on the right side)

Thermal Conductivity K_d = $30 \frac{J}{msK}$ (material on the left side)

Specific heat C_p = $2.0 \frac{J}{kgK}$ (for both materials)

Grid size d = 0.1 m

- **Process Parameters:**

Contact conductance coefficient h = $10 \frac{J}{m^2sK}$

Initial temperature T_C = 1000 K (the material on the right side)

Initial temperature T_D = 20 K (the material on the left side)

Time step size t $=0.0001 \text{ s}$

Time step n $=200$

Total time is 0.02 s

• **Boundary conditions:**

Temperature at point 1 $T_1 = 20 \text{ K}$

Temperature at point 5 $T_5 = 1000 \text{ K}$

After 200 time steps, we get the temperature distribution along line shown in figure (4.8).

Table 1 shows the result of LeVeque's method. We see that the method gives the jump across the point α accurately. Also, we can compare our numerical results to the exact solution in table 1

Figure 4.8: Temperature distribution after 200 time steps

<i>n</i>	<i>exact solution</i>	<i>numerical solution</i>	<i>Error</i>
1	20	20	0
2	49.14498	49.1449	8×10^{-5}
3	78.28996	78.2898	1.6×10^{-4}
4	978.14126	978.141	2.6×10^{-4}
5	1000	1000	0

Table 1 Numerical results for case study one

The Maximum error over all grid points is:

$$||E_n|| = \max_{i,j} |u(x_i, y_j) - u_{i,j}|$$

$u_{i,j}$ is the computed approximation at the grid points (x_i, y_j) . Local truncation errors $O(h^2)$ are expected at those points 3 and 4 which are close to the interface.

4.3.2 Case study 2: *Two-dimensional test case*

Steady case:

For the first test in the two dimensional case, the steady case with Dirichlet boundary conditions is used as shown in Figure (4.10).

T1	T2	T3	T4	T5	T6	T7	T8
T1							T8
T1							T8
T1							T8
T1							T8
T1							T8
T1							T8
T1	T2	T3	T4	T5	T6	T7	T8

Figure 4.9: Steady case:

- Geometry and parts:

8x8 square with element size 1m x 1m

- Material property:

Thermal Conductance: $\kappa = 1 \text{ W/m} \cdot \text{C}^\circ$

- Boundary conditions:

$T_1 = 100 \text{ K}$, $T_2 = 200 \text{ K}$, $T_3 = 300 \text{ K}$, $T_4 = 400 \text{ K}$, $T_5 = 500 \text{ K}$,

$T_6 = 600 \text{ K}$, $T_7 = 700 \text{ K}$, $T_8 = 800 \text{ K}$

- The expected result:

There is no flux along the y direction, so the problem can be treated as a one dimensional problem. The temperature distribution will be

linear along the x direction.

- The obtained result:

Figure 4.10: Temperature distribution in steady case:

The obtained result has been shown in figure (4.10) for each layer along the x direction. The obtained result is the same as expected.

Transient case:

1. Test 1: Constant initial temperature:

B	B	B	B	B	B	B	B
B	T	T	T	T	T	T	B
B	T	T	T	T	T	T	B
B	T	T	T	T	T	T	B
B	T	T	T	T	T	T	B
B	T	T	T	T	T	T	B
B	T	T	T	T	T	T	B
B	B	B	B	B	B	B	B

Figure 4.11: Test with constant initial temperature case

In this test, the boundary condition is prescribed as insulated and the initial condition is prescribed as a constant temperature T , as shown in Figure (4.11) (B is the node type which is a prescribed boundary condition, and T is the node type which is prescribed the initial temperature condition). All the properties and physical parameters are used as follows:

- Geometry and parts:

8x8 square with element size 1m x 1m

- Material properties:

Specific heat: $C_p = 1100 \text{ J/kg} \cdot \text{C}^\circ$

Thermal Conductance: $\kappa = 1 \text{ W/m} \cdot \text{C}^\circ$

- Simulation properties:

Time step size=275 s

Time step=10

Total time =2750 s

- Boundary condition:

Flux $q = 0$

- Initial condition:

Constant temperature: $T=100\text{ K}$

- The expected result:

The temperature should not change with time.

- The obtained results:

The temperature T is kept at 100 K for every time step. The obtained result is the same as expected.

2. Test 2: Linear initial temperature:

In this test, the initial temperature of the nodes was modified as a linear function of the x value which is shown in figure (4.12). The following parameters were used.

B	B	B	B	B	B	B	B
B	T _x	T _x	T _x	T _x	T _x	T _x	B
B	T _x	T _x	T _x	T _x	T _x	T _x	B
B	T _x	T _x	T _x	T _x	T _x	T _x	B
B	T _x	T _x	T _x	T _x	T _x	T _x	B
B	T _x	T _x	T _x	T _x	T _x	T _x	B
B	T _x	T _x	T _x	T _x	T _x	T _x	B
B	T _x	T _x	T _x	T _x	T _x	T _x	B
B	B	B	B	B	B	B	B

Figure 4.12: Test with linear distributed temperature case

- Geometry and parts:

8x8 square with element size 1m x 1m

- Material properties:

Specific heat $C_p = 1100 \text{ J/kg} \cdot \text{C}^\circ$

Thermal Conductance: $\kappa = 1 \text{ W/m} \cdot \text{C}^\circ$

- Simulation properties:

Time step size=275s

Time step=10

Total time =2750s

- Boundary condition:

Flux $q = 0$

- Initial condition:

Prescribed linear temperature as: $T(x) = 100 \times (x - 0.5 \times dx)$

where dx is the mesh size, and x is the node coordinate value on the x direction.

- The expected result:

The total enthalphy, which defined as:

$$H = \sum_{t=0}^t C_p \times (T(t) - T(0))$$

should be conservative, where $T(t)$ is defined as the temperature at time t and $T(0)$ is defined as the initial temperature.

- The obtained results:

At each time step (from 0 to 15), the total enthalpy is zero. The obtained results are the same as expected results.

3. Test 3: Two different initial temperature prescribed between middle and sides of the square:

In this test, a initial temperature was prescribed between the middle

B	B	B	B	B	B	B	B
B	Tb	Tb	Tb	Tb	Tb	Tb	B
B	Tb	Tb	Tb	Tb	Tb	Tb	B
B	Tb	Tb	Ta	Ta	Tb	Tb	B
B	Tb	Tb	Ta	Ta	Tb	Tb	B
B	Tb	Tb	Tb	Tb	Tb	Tb	B
B	Tb	Tb	Tb	Tb	Tb	Tb	B
B	B	B	B	B	B	B	B

Figure 4.13: Different initial temperature case

of the square and the sides of the square, as shown in Figure (4.13).

- Geometry and parts:

8x8 square with element size 1mx1m

- Material property:

Specific heat: $C_p = 1100 \text{ J/kg} \cdot \text{C}^\circ$

Thermal Conductance: $\kappa = 1 \text{ W/m} \cdot \text{C}^\circ$

- Simulation properties:

Time step size=275 s

Time step=10

Total time =2750 s

- Boundary condition:

Flux $q = 0$

- Initial conditions:

As shown in the figure (4.13), $Ta = 900 \text{ K}$ and $Tb = 100 \text{ K}$.

- The expected result:

The total enthalpy where defined as:

$$H = \sum_{t=0}^t C_p * (T(t) - T(0))$$

should be conservative, which $T(t)$ is defined as the temperature at time t , and $T(0)$ is defined as the initial temperature.

- The obtained results:

At each time step (from 0 to 15), the total enthalpy is zero. The obtained result is the same as the expected result.

4. Test 4: Two dimensional case with simple embedded boundary

As in the one-dimensional case, the interface is extended from one point to a straight line as shown in Figure (4.14). The jump will happen in the normal direction of the interface (a straight line). The

Figure 4.14: Grids for the simple two dimension test case

same data are used as before:

- **Properties of the geometry and the Material:**

Thermal Conductivity: $K_c = 40 \frac{J}{msK}$ (material on the right side)

Thermal Conductivity $K_d = 30 \frac{J}{msK}$ (material on the left side)

Specific heat $C_p = 2.0 \frac{J}{kgK}$ (for both materials)

Grid size $d = 0.1$ m

- The equation for the interface is:

$$y = -4(x - 0.23) + 0.3$$

where y is the ordinant and x is the abscissa.

- **Process Parameters:**

Contact conductance coefficient: $h = 10 \frac{J}{m^2 s K}$

Initial temperature: $T_C = 1000 \text{ K}$ (the material on the right side of the interface)

Initial temperature: $T_D = 20 \text{ K}$ (the material on the left side of the interface)

Time step size: $t = 0.000005 \text{ s}$

Time step: $n = 200$

Total time: 0.001 s

- **Boundary conditions:**

Boundary conditions were prescribed as shown in Figure (4.14). The temperature on the left side of the interface was 1000K and temperature on the right side of the interface was 20K.

After 200 time steps, the temperature distribution on those nodes which are not coherent to the boundary is shown in Figure (4.15)

Figure 4.15: Temperature distribution after 200 time steps in simple 2D case

From Figure (4.15), a jump in temperature across the interface can be seen. With the line a-b in (4.14) becoming a vertical line, the exact solution can be obtained as in the one dimension problem.

5. Test 5: Two-dimensional case with circular embedded boundary

Based on the case with the simple embedded boundary, this is

Figure 4.16: A circle interface Γ in uniform grids

a more complicated case, as shown in Fig (4.16), which has an embedded boundary prescribed as a circle instead of a line. There are two separate cases that need to be considered:

- **Two-dimensional case with the circular embedded boundary using same materials**

In the first test, the same materials are used for both inside the circle and outside the circle. The parameters used are as follows:

– Geometry and parts:

8x8 square with element size $0.5m \times 0.5m, 0.25m \times 0.25m, 0.125m \times 0.125m$

The equation for the circle is: $(x - 4)^2 + (y - 4)^2 = 4$

– Material properties:

Specific heat: $C_p = 1000 \text{ J/kg.C}^\circ$

Thermal Conductance: $\kappa = 10 \text{ W/m.C}^\circ$

Contact Conductance: $h = 500 \text{ W/m}^2.\text{C}^\circ$

– Simulation properties:

Time step size = 6.25 s

Time step step = 10

Total time = 62.5 s

– Boundary condition:

Flux $q = 0$

– Initial condition:

Constant temperature: $T_{inside} = 930 \text{ K}$

Constant temperature: $T_{outside} = 300 \text{ K}$

– Expected result:

Before reach the steady state, the jump of temperature should be obtained near the embedded boundary.

– The obtained result:

The temperature distribution after nine time steps for the 16x16, 32x32 and 64x64 are shown by the contour plots (4.18) (4.20) and (4.22), also intersected surface plots (4.17) (4.19) and (4.21). From the plots, the jump can be seen near the embedded boundary as expected.

Figure 4.17: Temperature distribution on the intersected surface of 45 degree
for 16x16 mesh at ninth time steps for the same materials

Figure 4.18: Temperature distribution for 16x16 mesh at ninth time steps
for the same materials

Figure 4.19: Temperature distribution on the intersected surface of 45 degree
for 32x32 mesh at ninth time steps for the same materials

Figure 4.20: Temperature distribution for 32x32 mesh at ninth time steps
for the same materials

Figure 4.21: Temperature distribution on the intersected surface of 45 degree
for 64x64 mesh at ninth time steps for the same materials

Figure 4.22: Temperature distribution for 64x64 mesh at ninth time steps for the same materials

- **Two-dimensional case with the circle embedded boundary using the different materials**

In this test, two different materials are used for the parts inside the circle and outside the circle.

- Geometry and parts:

8x8 square with the element size: $0.5m \times 0.5m$ $0.25m \times 0.25m$
 $0.125m \times 0.125m$

The equation for the circle is : $(x - 4)^2 + (y - 4)^2 = 4$

- Material properties:

1. Material for the part inside the circle is AL380

Specific heat: $C_p = 1170 \text{ J/kg.C}^\circ$

Density: 2690 kg/m^3

Thermal conductivity is: $\kappa = 90 \text{ W/m.C}^\circ$

2. Material for the part outside the circle is silica⁷ Sand

Specific heat: $C_p = 1100 \text{ J/kg.C}^\circ$

Density: 1500 kg/m^3

Thermal conductivity is: $\kappa = 0.6 \text{ W/m.C}^\circ$

Contact Conductance: $h = 500 \text{ W/m}^2.\text{C}^\circ$

– Simulation properties:

Time step size = 687500 s

Time step = 10

Total time = 6875000 s

– Boundary condition:

Flux $q = 0$

– Initial conditions

Constant temperature: $T_{inside} = 930\text{ K}$

Constant temperature: $T_{outside} = 300\text{ K}$

– Expected result:

Before reaching steady state, a jump in temperature should be obtained near the embedded boundary.

– The obtained result:

The temperature distribution after nine time steps for the 16x16, 32x32 and 64x64 is shown by the contour plots (4.24) (4.26) and (4.28), also intersected surface plots (4.23) (4.25) and (4.27). From the plots, the jump can be seen near the embedded boundary, as expected, but an error comes out among the 16x16, 32x32 and 64x64 grids. This error evaluation will be left to the error analysis.

Figure 4.23: Temperature distribution on intersected surface of 45 degree for 16x16 mesh at third time steps with different materials

Figure 4.24: Temperature distribution for 16x16 mesh at ninth time steps with different materials

Figure 4.25: Temperature distribution on the intersected surface of 45 degree for 32x32 mesh at third time steps with different materials

Figure 4.26: Temperature distribution for 32x32 mesh at ninth time steps with different materials

Figure 4.27: Temperature distribution on the intersected surface of 45 degree for 64x64 mesh at third time steps with different materials

Figure 4.28: Temperature distribution for 64x64 mesh at ninth time steps with different materials

6. Test 6: Transient case versus steady case

This test is designed to prove the coherence between steady state and transient state analysis.

- Geometry and parts:

8x8 square with the element size: $0.5m \times 0.5m$ $0.25m \times 0.25m$ $0.125m \times 0.125m$

The equation for the circle is : $(x - 4)^2 + (y - 4)^2 = 4$

- Material properties:

1. Material for the part inside the circle is AL380

Specific heat: $C_p = 1170 \text{ J/kg.C}^\circ$

Density: 2690 kg/m^3

Thermal conductivity is: $\kappa = 90 \text{ W/m.C}^\circ$

2. Material for the part outside the circle is silica Sand

Specific heat: $C_p = 1100 \text{ J/kg.C}^\circ$

Density: 1500 kg/m^3

Thermal conductivity is: $\kappa = 0.6 \text{ W/m.C}^\circ$

Contact Conductance: $h = 500 \text{ W/m}^2.\text{C}^\circ$

- Simulation properties:

Time step size = 687500 s

Time step = 30 s

Total time = 2062500 s

- Boundary condition:

Flux $q = 0$

- Initial conditions

Constant temperature: $T_{inside} = 930\text{ K}$

Constant temperature: $T_{outside} = 300\text{ K}$

- Expected result:

The steady state should be reached and temperature become constant everywhere.

- The obtained result:

After 30 time steps, constant temperature was reached in three different meshes. The obtained results match the expected results.

Error Analysis

As mentioned at the end of last section, differences in temperature are obtained among the different meshes(16x16, 32x32 and 64x64), especially, in the metal parts. Also, the difference seems to changed with the time steps, as roughly shown in Fig (4.29)⁶

From the plot, one can see the error accumulating as the time step increases. It is desired to know where does this error come from? The most probable possibility is from the numerical error. In order to have the numerical stability, the minimal Fourier number⁷ should be larger or at least equal to 1. Because of the large difference between aluminum and sand, the Fourier Number is chosen equal to 1 corresponding to the sand material. However, in this case, the Fourier Number in the Aluminum part is almost 1024 in the 64x64 meshes, 256 in the 32x32 and 64 in 16x16, this will cause a large difference in temperature between the different meshes(64x64, 32x32 and 16x16).

⁶Here, we just compare the highest temperature in the metal, because the largest difference is in the metal part, but not in the sand part

⁷Fourier $u = \frac{\sigma \Delta t}{(\Delta L)^2}$

where $\sigma = \frac{\kappa}{C_p}$

Figure 4.29: The change of highest temperature between the 16x16 grids and 32x32 grids versus the time steps.

In order to verify validate this implementation of LeVeque's embedded theory, a test is designed to compare the two errors L1 and L2. which were defined as:

$$(4.3) \quad \begin{aligned} L1 &= \frac{\sum (T_{32} - T_{64})^2}{\sum (T_{64})^2} \\ L2 &= \frac{\sum (T_{16} - T_{64})^2}{\sum (T_{64})^2} \end{aligned}$$

where: T_{32} is the temperature in 32x32 mesh. T_{16} is the temperature in 16x16. T_{64} is the temperature in 64x64.

1. First, in this test case, it is necessary to generate 64x64, 32x32 and 16x16 grids such that the 16x16 grid is a subset of the 32x32 and 64x46 grids to get a set of same points(same x and y coordinate) in all the different meshes.
2. Then, one can use equation (4.3) to calculate the errors L1 and L2 using this set of data and compare them.

Here, different ways to pick up the nodes in 16x16, 32x32 and 64x64 are used to get a set of the same points.

- In the 16x16 case, the nodes are chosen to satisfy the equation

$$2dx + i \times 4 \times dx - 34dx$$

where dx is the distance between cell centers in the 64x64 grids

- In the 32x32 case, the nodes are chosen to satisfy the equation

$$dx + i \times 2 \times dx - 33dx$$

where dx is the the distance between cell centers in the 64x64 grids

- In the 64x64 case, the nodes are chosen to satisfy the equation

$$dx + i \times dx - 33dx$$

where dx is the the distance between cell centers in the 64x64 grids

In this way, one obtains 15x15 nodes which have the same x and y coordinates among the three different meshes. Using equation (4.3) to calculate the errors at the ninth time step, we obtain:

$$L1 = 0.048196$$

and

$$L2 = 0.014644$$

$$\text{Ratio} = \frac{L1}{L2} = 3.3$$

A ratio of 4 indicates second-order accuracy. From the above numerical result, this implementation LeVeque's method has been validated least for these tests.

Chapter 5

Conclusions

5.1 Conclusion

The work presented here uses using Levque's immersed or embedded interface method to solve the Energy equation for both transient and steady cases. Instead of solving the complicated geometry interface problem, the immersed interface method just tries to embed the whole interface into a simple domain and uses a finite different method on a regular grid.

It is shown that to get the discontinuous coefficients for the points close to the interface is by requiring all the terms in the truncation expression

to vanish except the second-order error term. In this way, the second-order accuracy can be obtained in the numerical solution of the Energy equation with the discontinuous coefficients.

Several case studies in one dimensional and two dimensional problems show the results of using the LeVeque's method. Also, a quadratic error is obtained while the mesh size doubled. This implementation of LeVeque's immersed method is validated for these tests as a more accurate numerical method to solve the partial differential equations with an irregular surface Γ of codimension 1 contained in a domain Ω .

5.2 Recommendations for Future Work

The work that has been done here can be extended in future work as follows:

- The two dimensional analysis should be extended to three dimensions.

This will enable modelling of more complicated 3-d geometry.

- The present work assumes there is no heat source. The more sophisticated case could be extended to include a constant heat source as well as a heat source with a discontinuous function.
- LeVeque's algorithm assumed that no points on the interface coincide with the grid points, but just cut between grid points. More work is needed to consider the case which the points on the interface intersects one or more grid points.

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Appendix

In a two dimensional problem, the variables in local coordinates can be written as η and η . We define the parametric equation for the χ and ξ to be : $\xi = \chi(\eta)$, $\eta = \eta$. Here we will derive χ'' in the circle case as follows:
Let us define the equation for the circle:

$$x^2 + y^2 = R^2$$

The transformation to local coordinates is

$$(.1) \quad \xi = (x - x^*) \cos \theta + (y - y^*) \sin \theta$$

$$(.2) \quad \eta = -(x - x^*) \sin \theta + (y - y^*) \cos \theta$$

equation (.1) $x \sin \theta +$ equation (.2) $x \cos \theta$ And :
(equation (.1)) $x \cos \theta -$ (equation (.2)) $x \sin \theta$, we get

$$\xi \sin \theta + \eta \cos \theta = y - y^*$$

$$(.3) \quad \eta \cos \theta - \xi \sin \theta = x - x^*$$

where x^* and y^* is a point on the interface. and $R^2 - (x^*)^2 - (y^*)^2 = 0$

Because it satisfies the equation $x^2 + y^2 = R^2$. so

$$(\xi \sin \theta + \eta \cos \theta + y^*)^2 + (\xi \cos \theta - \eta \sin \theta + x^*)^2 = R^2$$

Expanding it, we get:

$$\xi^2 + \eta^2 + 2\xi(y^* \sin \theta + x^* \cos \theta) + 2\eta(y^* \cos \theta - x^* \sin \theta) = R^2 - (x^*)^2 - (y^*)^2$$

$$\xi^2 + \eta^2 + 2\xi(y^* \sin \theta + x^* \cos \theta) + 2\eta(y^* \cos \theta - x^* \sin \theta) = 0$$

Differentiate with respect to η

$$2\xi\xi' + 2\eta + 2(y^* \sin \theta + x^* \cos \theta)\xi' + 2(y^* \cos \theta - x^* \sin \theta) = 0$$

Here $(y^* \cos \theta - x^* \sin \theta) = 0$

Now differentiate this equation with respect to η again

$$2\xi\xi' + 2\xi\xi'' + 2\xi''(y^* \sin \theta + x^* \cos \theta) = 0$$

Because $\xi' = 0, \xi = 0$ at point (x^*, y^*) , so

$$\begin{aligned}\xi'' = \chi'' &= \frac{-1}{\xi + (y^* \sin \theta + x^* \cos \theta)} \\ &= \frac{-1}{(y^* \sin \theta + x^* \cos \theta)} = \frac{-1}{((x^*)^2 + (y^*)^2)^{\frac{1}{2}}}\end{aligned}$$

IMAGE EVALUATION TEST TARGET (QA-3)

APPLIED IMAGE, Inc.
1653 East Main Street
Rochester, NY 14609 USA
Phone: 716/482-0300
Fax: 716/288-5989

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