

Diffusion

(February 3, 2002)

We start by looking at 1D diffusion, e.g. the 1D heat conduction equation (see Eq. 4.3 V & M)

$$\frac{d}{dx} \left(k \frac{dT}{dx} \right) + S = 0.$$

To discretize (i.e. to go from a *continuous* differential equation to an algebraic *discrete* equation) this equation is integrated over a control volume (C.V.), see figure below

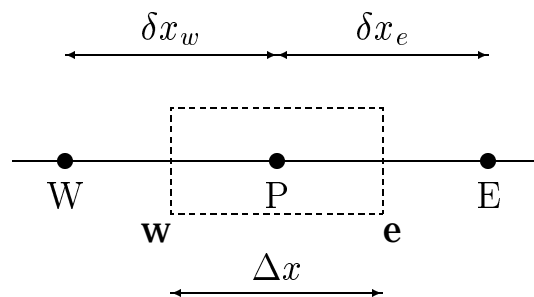


Figure 1D control volume. Node P located in the middle of the control volume.

$$\int_w^e \left[\frac{d}{dx} \left(k \frac{dT}{dx} \right) + S \right] dx = \left(k \frac{dT}{dx} \right)_e - \left(k \frac{dT}{dx} \right)_w + \bar{S} \Delta x = 0 \quad (1)$$

where (see the figure above):

P: an arbitrary node

E, W: its east and west neighbour node, respectively

e, w: the control volume's east and west face, respectively

\bar{S} : volume average of S

The temperature T and the coefficient of heat conductivity k are stored at the nodes W , P and E . Now we need the derivatives dT/dx at the faces w and e . These are estimated from a straight line connecting the two adjacent nodes, i.e.

$$\left(\frac{dT}{dx}\right)_e \simeq \frac{T_E - T_P}{\delta x_e}, \quad \left(\frac{dT}{dx}\right)_w \simeq \frac{T_P - T_W}{\delta x_w}. \quad (2)$$

These expressions are second-order accurate. This will now be shown using Taylor expansion. We want to show how exact the expression

$$\begin{aligned} \frac{1}{\Delta x} \int \frac{d^2 T}{dx^2} dx &= \frac{1}{\Delta x} \left[\left(\frac{dT}{dx}\right)_e - \left(\frac{dT}{dx}\right)_w \right] \\ &\simeq \frac{1}{\Delta x} \left(\frac{T_E - T_P}{\Delta x} - \frac{T_P - T_W}{\Delta x} \right) = \frac{1}{(\Delta x)^2} (T_E - 2T_P + T_W), \end{aligned} \quad (3)$$

is. Note that we have assumed that $\Delta x = \delta x_w = \delta x_e$ (otherwise, the method is actually not second-order accurate). Taylor expansion gives

$$\begin{aligned} T_E &= T_P + \Delta x \left(\frac{dT}{dx}\right)_P + \frac{(\Delta x)^2}{2} \left(\frac{d^2 T}{dx^2}\right)_P + \frac{(\Delta x)^3}{6} \left(\frac{d^3 T}{dx^3}\right)_P \\ &\quad + \frac{(\Delta x)^4}{12} \left(\frac{d^4 T}{dx^4}\right)_P + \dots \\ T_W &= T_P - \Delta x \left(\frac{dT}{dx}\right)_P + \frac{(\Delta x)^2}{2} \left(\frac{d^2 T}{dx^2}\right)_P - \frac{(\Delta x)^3}{6} \left(\frac{d^3 T}{dx^3}\right)_P \\ &\quad + \frac{(\Delta x)^4}{12} \left(\frac{d^4 T}{dx^4}\right)_P + \dots \end{aligned} \quad (4)$$

Eqs. 3 and 4 now give

$$\begin{aligned}\frac{1}{\Delta x} \int \frac{d^2 T}{dx^2} dx &= \frac{1}{(\Delta x)^2} (T_E - 2T_P + T_W) + \mathcal{O}((\Delta x)^2) \\ &= \left(\frac{d^2 T}{dx^2} \right)_P + \frac{1}{6} \left(\frac{d^4 T}{dx^4} \right)_P (\Delta x)^2 + \dots\end{aligned}$$

which is wanted we wanted to show.

The heat conductivity k is also needed at the faces. It is estimated by linear interpolation between the adjacent nodes. For the east face, for example, we obtain

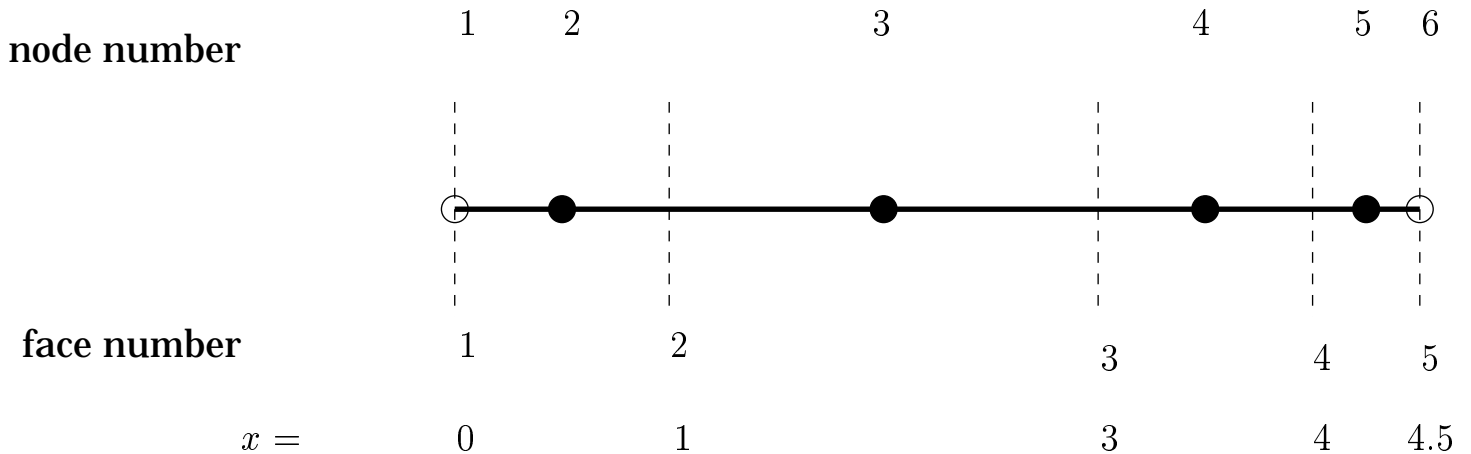
$$k_e = f_x k_E + (1 - f_x) k_P, \quad f_x = \frac{0.5 \Delta x}{\delta x_e}. \quad (5)$$

For an equidistant mesh (constant $\Delta x \Rightarrow \Delta x = \delta x_w = \delta x_e$) $f_x = 0.5$.

Insertion of Eq. 2 into Eq. 1 gives (see Eq. 4.11 in V & M)

$$\begin{aligned}a_P T_P &= a_E T_E + a_W T_W + S_U \\ a_E &= \frac{k_e}{\delta x_e}, \quad a_W = \frac{k_w}{\delta x_w}, \quad S_U = \bar{S} \Delta x, \quad a_P = a_E + a_W\end{aligned} \quad (6)$$

AN EXAMPLE



Constant heat source/unit length, $S = 2$; $k = \text{constant} = 1$; $T(0) = T_1 = 1$; $T(4.5) = T_6 = 10$.

Node 2

$$a_{E,2} = \frac{k_e}{1.5} = \frac{1}{1.5} = \frac{2}{3}, \quad a_{W,2} = \frac{k_w}{0.5} = \frac{1}{0.5} = 2, \quad S_{U,2} = 2 \cdot 1 = 2$$

$$a_{P,2} = a_{E,2} + a_{W,2} = \frac{8}{3}$$

We get the following equation for node 2:

$$\boxed{\frac{8}{3}T_2 = 2T_1 + \frac{2}{3}T_3 + 2} \quad (7)$$

Node 3

$$a_{E,3} = \frac{1}{1.5} = \frac{2}{3}, \quad a_{W,3} = \frac{1}{1.5} = \frac{2}{3}, \quad S_{U,3} = 2 \cdot 2 = 4$$
$$a_{P,3} = a_{E,3} + a_{W,3} = \frac{4}{3}$$

We get the following equation for node 3:

$$\boxed{\frac{4}{3}T_3 = \frac{2}{3}T_2 + \frac{2}{3}T_4 + 4} \quad (8)$$

Node 4

$$a_{E,4} = \frac{1}{0.75} = \frac{4}{3}, \quad a_{W,4} = \frac{1}{1.5} = \frac{2}{3}, \quad S_{U,4} = 2 \cdot 1 = 2$$
$$a_{P,4} = a_{E,4} + a_{W,4} = 2$$

We get the following equation for node 4:

$$\boxed{2T_4 = \frac{2}{3}T_3 + \frac{4}{3}T_5 + 2} \quad (9)$$

Node 5

$$a_{E,5} = \frac{1}{0.25} = 4, \quad a_{W,5} = \frac{1}{0.75} = \frac{4}{3}, \quad S_{U,5} = 2 \cdot 0.5 = 1$$
$$a_{P,5} = a_{E,5} + a_{W,5} = \frac{16}{3}$$

We get the following equation for node 5:

$$\boxed{\frac{16}{3}T_5 = \frac{4}{3}T_4 + 4T_6 + 1} \quad (10)$$

Equations 7–10 can be written on matrix form

$$\begin{pmatrix} 8/3 & -2/3 & 0 & 0 \\ -2/3 & 4/3 & -2/3 & 0 \\ 0 & -2/3 & 2 & -4/3 \\ 0 & 0 & -4/3 & 16/3 \end{pmatrix} \begin{pmatrix} T_2 \\ T_3 \\ T_4 \\ T_5 \end{pmatrix} = \begin{pmatrix} 2 \cdot 1 + 2 \\ 4 \\ 2 \\ 4 \cdot 10 + 1 \end{pmatrix} \quad (11)$$

This equation system can easily be solved by inverting the matrix. However, in CFD (Computational Fluid Dynamics) the equation systems are never (except in very special cases) solved by matrix inversion, because of two reasons:

- 1) for a large problem, the number of grid nodes can be well over 1 million, which gives a matrix of $10^6 \times 10^6$ to invert. Storage requirement for such a matrix would be 4×10^{12} bytes = 4000 GB, which exceeds the capacity of any existing supercomputer;
- 2) for fluid flow, which is governed by the Navier-Stokes equations, the equations are non-linear, which means that one would need to iterate anyway.

Instead of matrix inversion, iterative solvers are used. The simplest solver is the Gauss-Seidel solver. A more efficient solver is TDMA (see Chapter 7 in V & M). In this

example we use the Gauss-Seidel solver. In this solver the discretized equation (Eq. 6) is rewritten as

$$T_P = \frac{a_E T_E + a_W T_W + S_U}{a_P}.$$

For Eqs. 7–10 we get

$$\begin{aligned} T_2 &= (2T_1 + 2/3T_3 + 2)/(8/3) \\ T_3 &= (2/3T_2 + 2/3T_4 + 4)/(4/3) \\ T_4 &= (2/3T_3 + 4/3T_5 + 2)/2 \\ T_5 &= (4/3T_4 + 4T_6 + 1)/(16/3) \end{aligned} \tag{12}$$

Iteration 1

We start by computing T_2 . As we don't have any value for T_3 we have to guess one; for simplicity we set $T_3 = 0$, which gives

$$T_2 = (2 \cdot 1 + 2/3 \cdot 0 + 2)/(8/3) = 1.5$$

When computing T_3 , we use the recent computed value for T_2 , and we set $T_4 = 0$, so that

$$T_3 = (2/3 \cdot 1.5 + 2/3 \cdot 0 + 4)/(4/3) = 3.75$$

When computing T_4 and T_5 , we proceed in the same way

$$T_4 = (2/3 \cdot 3.75 + 4/3 \cdot 0 + 2)/2 = 2.25$$

$$T_5 = (4/3 \cdot 2.25 + 4 \cdot 10 + 1)/(16/3) = 8.25$$

where we've used the boundary value of $T_6 (= 10)$.

Iteration 2

$$T_2 = 2.44, T_3 = 5.34, T_4 = 8.28, T_5 = 9.76$$

Iteration 3

$$T_2 = 2.84, T_3 = 8.56, T_4 = 10.36, T_5 = 10.28$$

⋮

Iteration 13

$$T_2 = 4.2498, T_3 = 10.9997, T_4 = 11.7498, T_5 = 10.62496$$

Iteration 14

$$T_2 = 4.2499, T_3 = 10.9999, T_4 = 11.7499, T_5 = 10.62498$$

The differential equation for our example reads

$$t'' + 2 = 0, t(x = 0) = 1, t(x = 4.5) = 10$$

which has the solution

$$t = 6.5x - x^2 + 1.$$

The exact solution at the nodes is:

$$t(x = 0.5) = 4, t(x = 2) = 10$$
$$t(x = 3.5) = 11.5, t(x = 4.25) = 10.5625$$

In this example we find that with the Gauss-Seidel solver we find an approximate solution to Eq. 11 after approximately 13 iterations. However, it could be sufficient to stop

the iteration procedure after, say, 8 iterations; or, maybe, we want to solve Eq. 11 very accurately, and need to do 20 iterations. It is clear that we need some kind of convergence criterion.

Convergence Criteria

Compute the residual for Eq. 6

$$R = \sum_{\text{all cells}} |a_E T_E + a_W T_W + S_U - a_P T_P|$$

Since we want Eq. 6 to be satisfied, the difference of the right-hand side and the left-hand side is a good measure of how well the equation is satisfied. Note that R has the units of the integrated differential equation. Thus, in the present case R has the same dimension as heat transfer rate, i.e. Joule per second $[J/s] = [W]$. If $R = 1[W]$, it means that the residual for the computation is 1. This does not tell us anything, since it is problem dependent. We can have a problem where the total heat transfer rate is $1000[W]$, and a another where it is only $1[W]$. In the former case $R = 1$ means that the solutions can be considered converged, but in the latter case this is not true at all. We realize that we must normalize the residual to be able to judge whether the equation system has converged or not. The criterion for convergence is then

$$\frac{R}{F} \leq \varepsilon$$

where $0.0001 < \varepsilon < 0.01$, and F represents the total flux of T , i.e. total heat transfer rate.

Regardless if we solve the continuity equation, the Navier-Stokes equation or the energy equation, the procedure is

the same: F should represent the total flux of the dependent variable.

- Continuity equation. F is here the total incoming mass flux \dot{m} .
- Navier-Stokes equation. The unit is that of a force, i.e. Newton. A suitable value of F is obtained from $F = \dot{m}U$ at the inlet.
- Energy equation. F should be the total incoming heat flux. In a convection-diffusion problem we can take the convective flux at the inlet i.e. $F = \dot{m}c_p T$. In a conduction problem we can integrate the boundary flux, taking the absolute value at each cell, since the sum will be zero in case of internal source. If there are large heat sources in the computational domain, F could be taken as the sum of all heat sources.

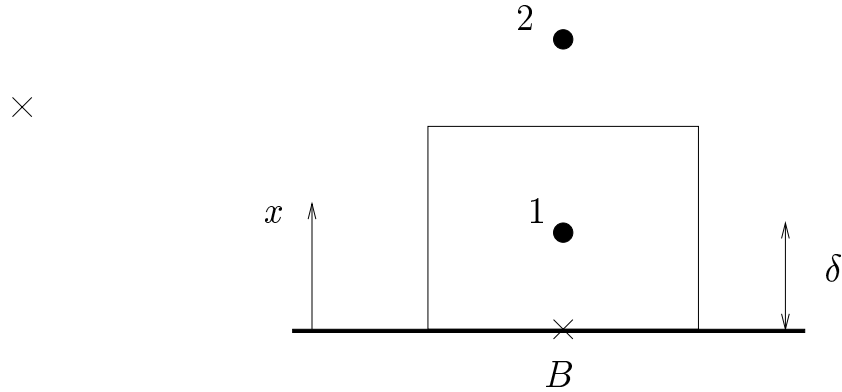
Boundary Conditions

The general source S is expressed as

$$S = S_P \Phi_P + S_U$$

where Φ is the general variable ($\Phi = U, V, T$, etc.).

Sometimes boundary conditions are introduced via the source term.



The discretized equation with the general source term reads (cf. Eq. 6)

$$a_P T_P = a_E T_E + a_W T_W + S_U, \quad a_P = a_E + a_W - S_P$$

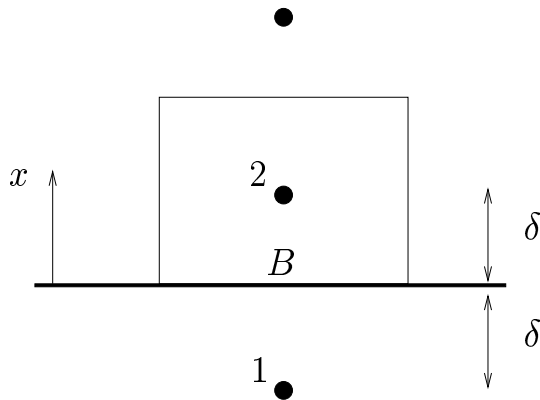
where E and W denote east and west, respectively. Now we want to introduce the boundary conditions via S_U and S_P (cf. Example 4.1 p. 88 in V & M). We cut off the usual link between the node P and its west neighbour, T_0 (not shown in the figure above) by setting $a_W = 0$. We can write the equation above for node 1 as

$$a_{P,1} T_1 = a_{E,1} T_2 + 0 + S_{U,1}, \quad a_{P,1} = a_{E,1} + 0 - S_{P,1} \quad (13)$$

Identification of Eqs. 13 and 6 gives

$$S_{P,1} = -a_{W,1}^{old} = -\frac{k_B}{\delta}, \quad S_U = a_{W,1}^{old} T_B = \frac{k_B}{\delta} T_B$$

Sometimes, the boundary node is stored half a control volume *outside* the computational domain, see figure below.



The value at the boundary B is known, but not at node 1. We mirror the variable around the boundary plane, i.e.

$$T_B = \frac{1}{2}(T_1 + T_2) \Rightarrow T_1 = 2T_B - T_2$$

where T_B is known and T_2 is taken at its most recent computed value (as in the Gauss-Seidel solver).

For setting homogeneous Neumann boundary conditions (i.e. $\partial T / \partial x = 0$), there are two different ways.

1. Explicit

The most obvious way is to set $T_1 = T_2$ (see figure above) after each iteration so that $\partial T / \partial x = 0$. When the equation system is converged $T_1^{n+1} = T_2^{n+1} = T_2^n$, where $n + 1$ and n denote the present and previous iteration, respectively.

2. Implicit

A more efficient way is to manipulate the coefficient matrix. The 1D discretized heat conduction equation reads (see Eq. 6) without source term

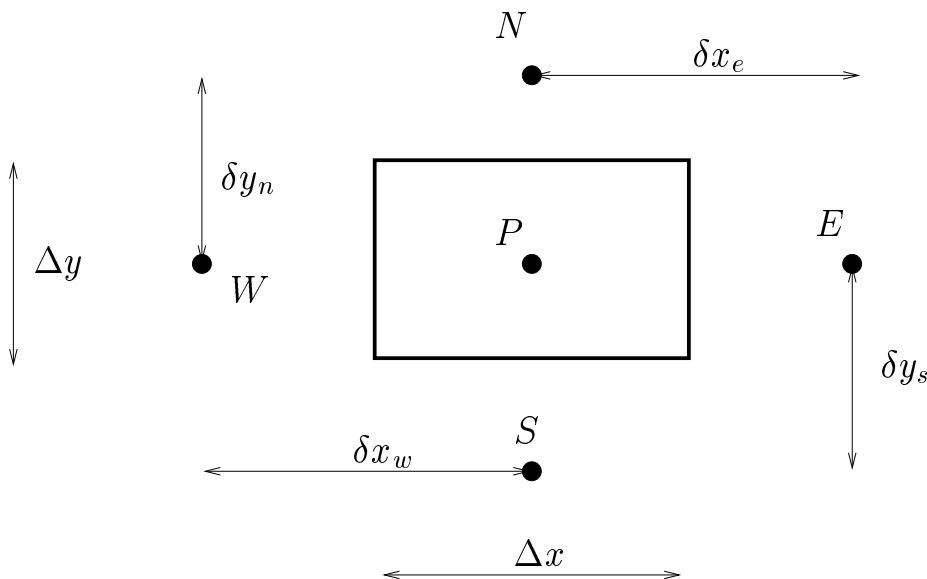
$$\begin{aligned} a_P T_P &= a_E T_E + a_W T_W \\ a_P &= a_E + a_W \end{aligned} \tag{14}$$

which can be rewritten as

$$0 = \underbrace{a_E(T_E - T_P)}_{-q_e} + \underbrace{a_W(T_W - T_P)}_{q_w}.$$

The equation expresses balance in diffusion of energy: what goes in, must come out. We want to set $\partial T/\partial x = 0$, which for the explicit procedure above was accomplished by setting $T_P = T_W$ (node 2 = node P) which gives $q_w = 0$ in the above equation. This can also be accomplished by setting $a_W = 0$. Note that this affects both the right-hand side (a_W) as well as the left-hand side (a_P) in Eq. 14.

2D Diffusion



The two-dimensional heat conduction equation reads (see Eq. 4.51 in V & M)

$$\frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k \frac{\partial T}{\partial y} \right) + S = 0. \quad (15)$$

In the same way as we did for the 1D case, we integrate over our control volume, but now it's in 2D (see the figure above), i.e.

$$\int_w^e \int_s^n \left[\frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k \frac{\partial T}{\partial y} \right) + S \right] dx dy = 0.$$

We start by the first term. The integration in x direction is carried out in exactly the same way as in 1D, i.e.

$$\begin{aligned} \int_w^e \int_s^n \left[\frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) \right] dx dy &= \int_s^n \left[\left(k \frac{\partial T}{\partial x} \right)_e - \left(k \frac{\partial T}{\partial x} \right)_w \right] dy \\ &= \int_s^n \left(k_e \frac{T_E - T_P}{\delta x_e} - k_w \frac{T_P - T_W}{\delta x_w} \right) dy \end{aligned}$$

Now integrate in the y direction. We do this by estimating the integral

$$\int_s^n f(y) dy = f_P \Delta y + \mathcal{O}((\Delta y)^2)$$

(i.e. f is taken at the mid-point P) which is second order accurate, since it is exact if f is a linear function. For our equation we get

$$\begin{aligned} \int_s^n \left(k_e \frac{T_E - T_P}{\delta x_e} - k_w \frac{T_P - T_W}{\delta x_w} \right) dy \\ = \left(k_e \frac{T_E - T_P}{\delta x_e} - k_w \frac{T_P - T_W}{\delta x_w} \right) \Delta y \end{aligned}$$

Doing the same for the diffusion term in the y direction in Eq. 15 gives

$$\begin{aligned} \left(k_e \frac{T_E - T_P}{\delta x_e} - k_w \frac{T_P - T_W}{\delta x_w} \right) \Delta y \\ + \left(k_n \frac{T_N - T_P}{\delta y_n} - k_s \frac{T_P - T_S}{\delta y_s} \right) \Delta x + \bar{S} \Delta x \Delta y = 0 \end{aligned}$$

Rewriting it as an algebraic equation for T_P , we get (see also Eq. 4.47 in V & M)

$$\begin{aligned} a_P T_P &= a_E T_E + a_W T_W + a_N T_N + a_S T_S + S_U \\ a_E &= \frac{k_e \Delta y}{\delta x_e}, \quad a_W = \frac{k_w \Delta y}{\delta x_w}, \quad a_N = \frac{k_n \Delta x}{\delta y_n}, \quad a_S = \frac{k_s \Delta x}{\delta y_s} \\ S_U &= \bar{S} \Delta x \Delta y, \quad a_P = a_E + a_W + a_N + a_S - S_P. \end{aligned} \tag{16}$$

In this 2D equation we have introduced the general form of the source term; this could also be done in the 1D equation (Eq. 6).