Heat Equation Notes

Mark Herndon

January 2023

Governing Equation

The unsteady heat equation is

$$\begin{aligned}\frac{\partial u}{\partial t} &= \alpha \nabla^2 u \\ &= \alpha \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right)\end{aligned}$$

where α is the thermal diffusivity

$$\alpha = \frac{k}{\rho c_p}, \qquad \left[\frac{L^2}{T} \right].$$

The finite-difference approximation is

$$\frac{u^{n+1}_{i,j,k} - u^n_{i,j,k}}{\Delta t} = \alpha \left(\delta_x^2 + \delta_y^2 + \delta_z^2 \right) \, u^n_{i,j,k}$$

where the central difference operators δ_i^2 are

$$\delta_x^2 u^n_{i,j,k} = \frac{u^n_{i-1,j,k} - 2u^n_{i,j,k} + u^n_{i+1,j,k}}{\Delta x^2}$$

$$\delta_y^2 u^n_{i,j,k} = \frac{u^n_{i,j-1,k} - 2u^n_{i,j,k} + u^n_{i,j+1,k}}{\Delta y^2}$$

$$\delta_z^2 u^n_{i,j,k} = \frac{u^n_{i,j,k-1} - 2u^n_{i,j,k} + u^n_{i,j,k+1}}{\Delta z^2}$$

Solution

The above three-dimensional equation is subject to boundary conditions at the start and end of the domain in each direction, where we can specify temperature (Dirichlet boundary condition)

$$\begin{aligned} u_{1,j,k} &= T_1, & u_{ni,j,k} &= T_2 \\ u_{i,1,k} &= T_3, & u_{i,nj,k} &= T_4 \\ u_{i,j,1} &= T_5, & u_{i,j,nk} &= T_6 \end{aligned}$$

or we can specify heat flux (Neumann boundary condition)

$$\begin{aligned}
-k\frac{\partial u_{1,j,k}}{\partial x} &= 0, \quad \text{(Perfectly insulated)} \\
-k\frac{\partial u_{ni,j,k}}{\partial x} &= 0, \quad \text{(Perfectly insulated)} \\
-k\frac{\partial u_{i,1,k}}{\partial x} &= 0, \quad \text{(Perfectly insulated)} \\
-k\frac{\partial u_{i,nj,k}}{\partial x} &= Q, \quad \text{(Heat source at top of cube)} \\
-k\frac{\partial u_{i,j,1}}{\partial x} &= 0, \quad \text{(Perfectly insulated)} \\
-k\frac{\partial u_{i,j,nk}}{\partial x} &= 0, \quad \text{(Perfectly insulated)}
\end{aligned}$$

and any combination of the above types. Note that the heat flux condition requires the thermal conductivity, *not* diffusivity.

Neumann boundary conditions are applied by either first order forward or backward difference at the boundary, for example,

$$\begin{aligned}
-k\frac{\partial u_{1,j,k}}{\partial x} &= 0 \\
\frac{u_{2,j,k} - u_{1,j,k}}{\Delta x} &= 0 \\
&\to u_{1,j,k} = u_{2,j,k}
\end{aligned}$$

or for a backward difference to a heat flux with a source term in the j-direction,

$$\begin{aligned}
-k\frac{\partial u_{i,nj,k}}{\partial x} &= Q \\
\frac{u_{i,nj,k} - u_{1,nj-1,k}}{\Delta y} &= -\frac{Q}{k} \\
&\to u_{i,nj,k} = u_{i,nj-1,k} - \Delta y\,\frac{Q}{k}
\end{aligned}$$

The solution to update your solution at $t = t + \Delta t$ is

$$u^{n+1}_{i,j,k} = u^n_{i,j,k} + \Delta t\alpha\left(\delta_x^2 + \delta_y^2 + \delta_z^2\right)\, u^n_{i,j,k}$$

where we typically loop through the interior points and then set end points based on boundary conditions. We can then modify this update procedure by knowing where our interfaces lie and modify the formula accordingly.

1 Interface

Assuming a grid point coincident with an interface, we will establish the condition for a perfect interface (we will orient this example in the j-direction, which aligns with y, and assumes layers are horizontal (width along x which thickness in y-direction). This implies

$$u^{lower}_{i,j,k} = u^{upper}_{i,j,k}$$

$$\alpha^{lower}\frac{\partial u^{lower}_{i,j,k}}{\partial y} = \alpha^{upper}\frac{\partial u^{upper}_{i,j,k}}{\partial y}$$

at j = index of interface. Taking backward different for the lower derivative and forward difference at the upper derivative (remember these points are coincident, just creating an equation here) we get

$$u_{i,j,k} - u_{i,j-1,k} = \frac{\alpha^{upper}}{\alpha^{lower}} \left(u_{i,j+1,k} - u_{i,j,k}\right)$$

$$\rightarrow u_{i,j,k} = \left(1 + \frac{\alpha^{upper}}{\alpha^{lower}}\right)^{-1} \left[u_{i,j-1,k} + \frac{\alpha^{upper}}{\alpha^{lower}} u_{i,j+1,k}\right].$$

For derivatives *parallel* and *coincident* to an interface boundary, we can perhaps take an average of the thermal diffusivities along that line and use the standard difference formulas... but that feels wrong! For a cube with planar materials and symmetric boundary conditions the problem reduces to one-dimensional, where you omit the spatial derivatives (and indices) of the 2 directions that do not vary in space.

Interfaces usually have a contact resistance and in fact have a *jump* in temperature from one material to the next, due to imperfect contact from surface roughness or other geometric properties. This example serves as a basic approximation to the problem. Contact resistances between materials are usually found experimentally, which then can be incorporated into the above algorithm.

A note on stability

For a Forward Euler solution, a criteria for numerical stability is the CFL condtion:

$$CFL = \alpha \frac{\Delta t}{\Delta x^2} \leq C_{max}$$

where we set $C_{max} = 1.0$. We can estimate an optimal time step for numeric stability be rearranging for our minimum spacing Δx and maximum thermal diffusivity α_{max}.