

The heat equation is a partial differential equation that describes many physical processes including conductive heat flow or the diffusion of an impurity in a motionless fluid.

In three-dimensional medium the heat equation is:

$$\frac{\partial u}{\partial t} = k \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right)$$

Here u is a function of (x, t, y, z) that represents temperature at time t at position (x, y, z)

The constant k depends on the material involved, it is called the thermal conductivity in the case of heat flow and diffusion coefficient in the case of diffusion. To simplify matters let us assume that the medium is one-dimensional. This could represent heat flow in a thin insulated wire or rod

Then partial differential equation becomes

$$\frac{\partial u}{\partial t} = k \frac{\partial^2 u}{\partial x^2}$$

where u is temperature at time t a distance x along the wire

$$u = u(x, t)$$

A finite difference solution

To solve this partial differential equation we need both initial conditions of the form $u(x, t = 0) = f(x)$, where $f(x)$ gives the temperature distribution in the wire at time 0, and boundary conditions at the endpoints of the wire, call them $x = a$ and $x = b$

We choose so-called Dirichlet boundary conditions

$u(x = a, t) = L_a; u(x = b, t) = L_b$ which correspond to the temperature being held steady at values L_a and L_b at the two endpoints

Though an exact solution is available in this scenario, let us instead illustrate the numerical method of finite differences.

To begin with, on computer we can only keep track of the temperature u at discrete set of times and discrete set of positions.

Let times be $0, \Delta t, 2\Delta t, \dots, n\Delta t$, and let the positions $a, a + \Delta x, \dots, J\Delta x = b$

let $u_j^n = u(a + J\Delta x, n\Delta t)$. Rewriting the partial differential equation in terms of finite-difference approximations to the derivatives, we get

$$\frac{\partial u}{\partial t} = \frac{u_j^{n+1} - u_j^n}{\Delta t};$$

$$k * \frac{\partial^2 u}{\partial x^2} = k * \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta x^2}$$

So we get

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = k * \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta x^2}$$

Thus if for a particular n , we know the values of u_j^n for all j we can solve equation above to find u_j^{n+1} for each j ;

$$u_j^{n+1} = u_j^n - \frac{k * \Delta t}{\Delta x^2} (u_{j+1}^n - 2u_j^n + u_{j-1}^n)$$

after some algebraic manipulation we get

$$u_j^{n+1} = (u_{j+1}^n - u_{j-1}^n) * l + (1 - 2 * l) * u_j^n$$

$$\text{where } l = \frac{k * \Delta t}{\Delta x^2}$$

In other words, this equation tells us how to find the temperature distribution at time step $n+1$ given the temperature distribution at time step n .

Thus our numerical implementation of the heat equation is a discretized version of the microscopic description of diffusion we gave initially, that heat energy spreads due to random interactions between nearby particles.