Computational Methods: Homework 1

D. J. Dean
Physics Division, Oak Ridge National Laboratory
P.O. Box 2008, Oak Ridge, TN 37831-6373 USA
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Homework is due on 10 February.

Heat equations describe the diffusion of heat in a material. Let $U(\vec{x},t)$ denote the temperature at a point $\vec{x}$ within a solid at time t. If we specify only one-dimensional flow, the heat equation is then given by

$$\frac{\partial}{\partial t}U(x,t) = \pm k\frac{\partial^2}{\partial x^2}U(x,t) \ , \tag{1}$$

where k is the thermall diffusivity of the material. This is a simple form of the equation of diffusion and may be extended to multi-dimensional objects. In a three-dimensional object the equation becomes $U_t = k(U_{xx} + U_{yy} + U_{zz}$. Details on the equation and its analytic solutions for certain problems can be found in Churchill's Operational Mathematics.

We would like to solve a simple diffusion problem. Let the temperature of the face of a semi-infinite solid $x \geq 0$ be a prescribed function $F(t)$ of time. If the initial temperature is zero, the temperature function $U(x,t)$ is the solution of the boundary value problem

$$U_t(x,t) = kU_{xx}(x,t) \qquad (x > 0, t > 0) \tag{2}$$

$$U(x,0) = 0 \qquad (x > 0) \tag{3}$$

$$U(0,t) = F(t) \ , \ \lim_{x\to\infty} U(x,t) = 0 \qquad (t > 0) \tag{4}$$

This problem has analytic solutions, but let's work on it with our knowledge of derivatives.

The diffusion equation is first order in time and second order in space. Let us define some grid points:

$$x_i = \frac{i}{I_{\max}}L \qquad \text{for} i = 0, 1, 2, \cdots, I_{\max} \tag{5}$$

$$t_n = \frac{n}{N_{\max}}T \qquad \text{for} n = 0, 1, 2, \cdots, N \tag{6}$$

where the our one dimensional bar is of length L and we are interested in time propagation up to time T. In a discrete form, it is given by

$$\frac{U(x_i,t_{n+1}) - U(x_i,t_n)}{\Delta t} = k\left\{\frac{U(x_{i+1},t_n) - 2U(x_i,t_n) + U(x_{i-1},t_n)}{(\Delta x)^2}\right\} \ . \tag{7}$$

This equation can be rearranged simply so that we can propagate in time

$$U(x_i,t_{n+1}) = \frac{k\Delta t}{(\Delta x)^2}\left[U(x_{i+1},t_n) - 2U(x_i,t_n) + U(x_{i-1},t_n)\right] + U(x_i,t_n) \ . \tag{8}$$

The flux through a given point (at the surface) is given by

$$\Phi(t) = -KU_x(0,t) \ , \tag{9}$$

while the total amount of heat that has been absorbed by the solid through a unit area of the face at time t is

$$Q(t) = \int_0^t \Phi(\tau)d\tau \ . \tag{10}$$

You will find a program in the directory /home/dean/class_573/chapter_I/programs/heat_eqn/heat_eqn.f90 that begins to solve this problem. You also need the input file, heat.input from the same directory. The code and a sample input file are also on the class web page as heat.tar.gz.

- You want to run the program with the input you have and see what kind of output you obtain. Use xmgrace to plot the heat flux at time t as a function of time. You can use $\kappa = 0.05$ and $K = 1.0$ throughout the heat equation part of the exercise.

- Now, keeping the length of the rod fixed, change Δx to see whether your results are numerically stable. You can do this by changing both the number of points N, the first number in the input, and Δx, the second number. Let's run the four cases, $N = 25$, $\Delta x = 0.4$, $N = 50$, $\Delta x = 0.2$, $N = 100$, $\Delta x = 0.1$, $N = 200$, $\Delta x = 0.05$, and $N = 400$ $\Delta x = 0.025$, $N = 800$, $\Delta x = 0.0125$. What can you say about convergence as you increase the number of grid points while keeping Δt a constant? You should plot the heat flux here. Don't plot the results that are numerically unstable, but state which ones are (or may be).

- Make a plot of the heat flux through the face of the solid as a function of time and repeat the same convergence studies as you did in the previous part of the exercise, except this time use $\Delta x = 0.025$, $N = 400$, and let $\Delta t = 0.1, 0.01, 0.001$, and the number of steps $N_t = 800, 8000, 80000$. How do these convergence plots look?

- Use $\Delta t = 0.001$, $N_t = 80000$, $\Delta x = 0.0125$ and $N = 800$. Now, modify your program such that the temperature on the face of the solid, governed by the function $F(t)$, is a sine wave with frequency ω (your driving function is then $F(t) = \sin(\omega t)$). For $N = 100$ and $\Delta x = 0.1$ make plots of $Q(t)$ when $\omega = 0.5, 1.0, 2.0$. At a fixed point, say at x_{20}, make a plot of the temperature as a function of time for the different values of ω. The temperature is going towards a constant value. What is it (you may have to run longer times to answer this one)?

- Modify your code to solve the wave equation with the Lax method. At time $t = 0$ set up a gaussian on the lattice with a width of 2.0. You may set $v = 1.0$, and use $N = 800$ $\Delta x = 0.01$, and $\Delta t = 0.001$, $N_t = 8000$. Plot what happens to u at x_{20}. What happens? You should make a plots of u(t) at times $N_t = 1, 1000, 2000, 3000, 4000, 8000$.

- Use your wave-equation code to show how the evolution becomes unstable if you choose $\frac{|v|\Delta t}{\Delta x}$ to be a greater than 1 (10), equal to 1, and below 1 (0.1). Show in a plot the behavior of u_{20} as a function of time. At what point in time do you begin to see problems with the solutions when the Courant condition is violated?