Tutorial

The Finite Difference method

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Contents

1 Introduction

This tutorial is intended to strengthen your understanding on the finite difference method (FDM). This technique will allow you to solve numerically many ordinary and partial differential equations.

To do the tutorial you must decompress the file `Sim_Meth_I_T4_11_12_Code.tar.gz` (use `tar -xvzf file_name`). You will find a set of folders containing the programs needed for each section.

2 Finite Difference Methods

Let's assume for simplicity our problem can be modeled using only time t and one spatial coordinate x . We further assume that space and time are discretized in intervals Δx and Δt respectively. Thus, the field $\Phi(x,t)$ can be written in its discretized version as

$$\Phi(i,j) \equiv \Phi(\ x\ =\ i\,\Delta x\ ,\ t\ =\ j\,\Delta t\ ). \tag{1}$$

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Given this notation, it is possible to write down partial derivatives of different order both in the forward, backward or centered schemes:

$$\left(\frac{\partial \Phi}{\partial x}\right)_{i,j} \approx \frac{\Phi(i \pm 1, j) - \Phi(i,j)}{\Delta x} + \mathcal{O}(\Delta x) \quad \text{(forward/backward)} \tag{2}$$

$$\left(\frac{\partial \Phi}{\partial t}\right)_{i,j} \approx \frac{\Phi(i, j \pm 1) - \Phi(i,j)}{\Delta t} + \mathcal{O}(\Delta t) \quad \text{(forward/backward)} \tag{3}$$

$$\left(\frac{\partial \Phi}{\partial x}\right)_{i,j} \approx \frac{\Phi(i + 1, j) - \Phi(i-1,j)}{2\ \Delta x} + \mathcal{O}(\Delta x^2) \quad \text{(centered)} \tag{4}$$

$$\left(\frac{\partial^2 \Phi}{\partial x^2}\right)_{i,j} \approx \frac{\Phi(i,j) - 2\ \Phi(i \pm 1, j) + \Phi(i \pm 2, j)}{(\Delta x)^2} + \mathcal{O}(\Delta x) \quad \text{(forward/backward)} \tag{5}$$

$$\left(\frac{\partial^2 \Phi}{\partial x^2}\right)_{i,j} \approx \frac{\Phi(i+1,j) - 2\ \Phi(i, j) + \Phi(i - 1, j)}{(\Delta x)^2} + \mathcal{O}(\Delta x^2) \quad \text{(centered)} \tag{6}$$

2.1 The diffusion equation (an example of parabolic PDE)

Let's suppose we have a rod of length $L = 2m$ which is initially at a temperature of $T = 473K$. Let's assume the rod is isolated except at the two ends ($x = 0$ and $x = L$). At time $t = 0$ we put the two ends in contact with an infinite reservoir of ice that keeps them constantly at a temperature of $273K$. We want to know how the temperature changes as a function of position and time.

The previous problem is related to solving the diffusion equation for the internal temperature $T(x, t)$

$$\alpha \frac{\partial^2 T}{\partial x^2} = \frac{\partial T}{\partial t}, \tag{7}$$

subject to boundary conditions

$$T(0, t) = 273K \tag{8}$$

$$T(2, t) = 273K \tag{9}$$

and to the initial condition

$$T(x, 0) = 473K. \tag{10}$$

In the previous equation α is the so-called *thermal diffusivity* (to know more, see for instance the Wikipedia:
`http://en.wikipedia.org/wiki/Heat_equation` and
`http://en.wikipedia.org/wiki/Thermal_diffusivity`.

There, you can find that for Carbon steel at 1% the thermal diffusivity is $\alpha = 1.172 \times 10^{-5} m^2/s$. Using the 1-point forward scheme for the time derivative, and the 2-points centered scheme for the second derivative in space, the diffusion equation can be written in its discretized form as:

$$T(i, j+1) = T(i, j) + r\left[T(i+1, j) - 2T(i,j) + T(i-1, j)\right] \tag{11}$$

where $r = \alpha \Delta t / \Delta x^2$. This is the Euler integration scheme (in time).

Homework 1 (4 points)

1. Modify the `C` code `example-finite-differences-1.c` to solve the previous problem. **Be careful**, two errors have been introduced in the C-Code. Plot the temperature profiles (T vs x) at $t = 1.0s,\ 10s,\ 100s,\ 1000s$ and $t = 10^5 s$. How does it look the stationary solution for this system?

2. How will the profile look like if the rightmost point of the rod is always maintained at $T = 473K$?

3. Is it possible to use any value for r? In case it is not possible, show an example illustrating what occurs. and try to explain why this happens? If you think it is possible to use any value of r, plot the temperature profiles using $\Delta x = 0.01$ and $\Delta t \geq 5$. Justify your answer.

4. The analytic solution to the symmetric problem is

$$T(x,t) = 273 + \frac{4(473-273)}{\pi} \sum_{k=0}^{k=\infty} \frac{1}{2k+1} \sin[(2k+1)\pi x/L] \exp[-\alpha t(2k+1)^2 \pi^2/L^2]. \tag{12}$$

   Check your numerical solutions against the exact solution. For a derivation of the previous analytical formula, see for instance A. N. Tikhonov and A. A. Samarskii, Equations of the Mathematical Physics, Pergamon Press, Oxford, 1963. Notice that previous formula converges fast for large values of t, while it converges extremely slow for small values of t.

2.2 The wave equation (an example of Hyperbolic PDE)

We want to solve the wave equation

$$\frac{\partial^2 \Phi}{\partial x^2} = \frac{1}{c^2} \frac{\partial^2 \Phi}{\partial t^2} \tag{13}$$

in the domain $0 < x < 1$ and for $t \geq 0$ subject to the initial conditions $\Phi(x,0) = sin(\pi\ x)$ and $\frac{\partial \Phi}{\partial t} = 0$ for $0 < x < 1$. The boundary conditions are $\Phi(0,t) = \Phi(1,t) = 0$.

Homework 2 (3 points)

1. Write the discretized wave equation using only centered differences, obtaining an expression that relates $\Phi(i, j+1)$ to $\Phi(i,j)$, $\Phi(i+1,j)$, $\Phi(i-1,j)$ and $\Phi(i,j-1)$.

2. Is there some trouble to modify the program `example-finite-differences-1.c` and get a solution for the PDE?

3. Solve the PDE using the modified formula for the initial time

$$\Phi(i,1) = (1-r)\Phi(i,0) + \frac{r}{2}\left[\Phi(i-1,0) + \Phi(i+1,0)\right] \tag{14}$$

where

$$r \equiv \left(\frac{c\Delta t}{\Delta x}\right)^2. \tag{15}$$

Can you explain how the previous starting formula is obtained? Hint: at the maximum of the oscillation, by definition it holds $\frac{\partial \Phi}{\partial t} = 0$.

4. Compare your numerical solution to the analytical solution

$$\Phi(x,t) = \sin(\pi x)\ \cos(\pi c t) \tag{16}$$

Which is the range of values of r suitable to get an accurate solution of the PDE? Can you justify why should be that the range of validity of r?

2.3 Poisson equation (an example of an elliptic PDE)

We want to solve the two-dimensional Poisson equation:

$$\frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2} = g(x,y). \tag{17}$$

If we use central differences, and for simplicity we set $\Delta x = \Delta y = h$ then we obtain

$$\Phi(i,j) = \frac{1}{4}\left[\Phi(i+1,j) + \Phi(i-1,j) + \Phi(i,j+1) + \Phi(i,j-1) - h^2 g(i,j)\right] \tag{18}$$

which leads to solving a system of algebraic equations of the style $[A][X] = [B]$ where $[X]$ are the unknown values, and $[B]$ is a column matrix containing the know values of Φ at the fixed nodes. There are several methods to find $[X]$ which becomes very tricky when we have many grid nodes because the matrices are in that case very large and it takes a lot of time to find numerically the solution. Here we will use a very simple method called successive over-relaxation (SOR) which basically consist on doing the following: we define the residual at node (i,j) as

$$R(i,j) \equiv \Phi(i+1,j) + \Phi(i-1,j) + \Phi(i,j+1) + \Phi(i,j-1) - 4\Phi(i,j) - h^2 g(i,j), \tag{19}$$

i.e., the amount by which Φ at point (i,j) does not satisfy the Poisson's equation. We iterate the process as follows, the $k+1$ iteration is obtained from the k iteration as

$$\Phi^{(k+1)}(i,j) \equiv \Phi^{(k)}(i,j) + \frac{\omega}{4} R^{(k)}(i,j) \tag{20}$$

the optimal value of the parameter ω, i.e. the one that speeds at maximum the convergence must be found by trial and error. When $\omega = 1$ the method is known as successive relaxation.

Let's suppose we want to solve the Poison equation in a square of size $L = 1$ using a grid of 10×10 nodes with boundary condition $\Phi = 0$ on the square border, and with a source term $g(x,y) = \text{const}$ within a circle or radius $1/4$;

Homework 3 (3 points)

1. Prove equation 18.

2. Use the `C` code `example-finite-differences-3.c` to solve the previous PDE. Try to use different mesh sizes (20, 50, 100,...)

3. How does the convergence time (use the `time` command) scales with increasing mesh size? Make a log-log plot of execution time versus mesh size and comment.

4. Change the value of ω for a fixed mesh size. How does the convergence time change?

3 To learn more

Suitable books to become more learned about FDM and FEM methods are:

- *Numerical Techniques in Electromagnetics*, Matthew N. O. Sadiku. CRC Press (2001). ISBN: 0-8493-1395-3.