Simulationsmethoden I WS 09 10

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 `tutorial-finite-diff.tar` (use `tar -xzf file\_name`). You will find a set of folders containing the programs needed for each section. **BE CAREFUL**, errors have been introduced in the C-Codes, which you should fix.

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:

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

$$\left(\frac{\partial \Phi}{\partial t}\right)_{i,j} \approx \frac{\Phi(i, j \pm 1) - \Phi(i,j)}{\Delta t} + \mathcal{O}(\Delta 2) \quad \text{(forward/backward)} \tag{3}$$

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

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

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

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).

Tasks

1. Modify the `C` code `example-finite-differences-1.c` to solve the previous problem. 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.

5. Derive the discretized heat equation using only forward and backward schemes.

6. Implement the above derived scheme to solve the symmetric heated bar problem. Notice that in this case you should modify slightly your boundary conditions. Comment the results you obtain, and compare them to the results obtained with the central difference scheme.

2.2 The wave equation (an example of Hyperbolic PDE)

We want to solve the wave equation

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

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 $\Phi(0,t) = \Phi(1,t) = 0$.

Tasks

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 "./sources/example-finite-differences-1.c" and get a solution for the PDE?

3. Try to solve the PDE using the starting formula

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

where

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

Can you explain how the previous starting formula is obtained? **Hint: we recommend you to use r=1 to solve the PDE, as you can see many terms will then simplify.**

4. Compare your numerical solution to the analytical solution

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

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

2.3 The Poisson's equation (an example of Elliptic PDE)

Let's suppose we want to solve the following two-dimensional Poisson's 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 colum 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 matrixes 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. Alternatively, in order to speed calculations, one can use for the iterations

$$\begin{aligned} \Phi^{(k+1)}(i,j) \quad \equiv \quad & \Phi^{(k)}(i,j) + \frac{\omega}{4}\Big[\Phi^{(k)}(i+1,j) + \Phi^{(k+1)}(i-1,j) + \Phi^{(k)}(i,j+1) \\ & + \Phi^{(k+1)}(i,j-1) - 4\Phi^{(k)}(i,j) - h^2 g(i,j)\Big] \end{aligned} \tag{21}$$

When this last expression is used, it is known that the optimal value of $\omega \in [1, 2]$.

Let's suppose we want to solve the Poison equation in square of size $L = 1$ using a grid of 5×5 nodes ($i \in [0, 4]$, and $j \in [0, 4]$], where the following boundary conditions exist:

$$\begin{aligned}
\Phi(i, 0) &= 0 \quad for\ i = 1, 2, 3 \\
\Phi(i, 4) &= 20 \quad for\ i = 1, 2, 3 \\
\Phi(0, j) &= -10\ for\ j = 1, 2, 3 \\
\Phi(4, j) &= +10\ for\ j = 1, 2, 3 \\
\Phi(0, 0) &= -5 \\
\Phi(4, 0) &= +5 \\
\Phi(0, 4) &= +5 \\
\Phi(4, 4) &= +15
\end{aligned}$$

and $g(x, y) = x\ (y - 1)$.

Tasks

1. Proof equation 18.

2. Use the c code "./sources/example-finite-differences-3.c" to solve the previous PDE. Is there some difference in the values of ω one can use when using eq. 21 or eq. 20.

3. Refine the mesh to $N \times N$ grid points , with $N = 5, 10, 20, 50, 100, 500, 1000$. Use the eq. 21 to do the calculations. When N increases, you get convergence faster or slower (try to tune w to an optimal value by trial and error) ? Compare ω values you have found with the theoretical prediction that states that when using eq. 21 in a rectangular region, the optimum over-relaxation factor is given by the smaller root of the equation: $t^2\ \omega^2 - 16\ \omega + 16 = 0$ where $t = cos(\pi/N_x) + cos(\pi/N_y)$ and $N_x = N_y = N$ in the case of a square region. How does the time needed to solve the equation evolve with N. **Hint: use the command *"time"*** .

4. Check your numerical solution against the know exact solution given in the following table:

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.

Table 1: Values for the exact solution

x	y	Exact Value
1/4	1/4	-3.429
1/4	2/4	-2.029
1/4	3/4	4.277
2/4	1/4	-0.1182
2/4	2/4	2.913
2/4	3/4	9.593
3/4	1/4	2.902
3/4	2/4	6.065
3/4	3/4	11.13