LIÈGE université
Sciences Appliquées

Lecture 3b Computation of Solutions

Mathématiques appliquées (MATH0504-1)

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Numerical solutions of PDEs

- We have found formulae for solutions to several first and second order PDEs, but other problems encountered in practice are not as simple and cannot be solved by formulae
- Even when there is a formula, it might be so complicated that we would prefer to visualize a typical solution by looking at its graph
- Let us start investigating if we can reduce the process of solving a PDE with its auxiliary conditions to a finite number of arithmetic calculations that can be carried out by computer

Numerical solutions of PDEs

There are dangers in doing so:

- If the numerical method is not carefully designed, the computed solution may substantially differ from the actual one.
- For difficult problems the computation could easily take so long (years…) that it would not be tractable

Two well known numerical methods are Finite Difference (FD) and Finite Element (FE): we will introduce both.

Finite Volume (FV) is another numerical method, widely used in fluid flow computations.

Learning objectives of this class

Review elementary finite difference (FD) schemes

Become aware the dangers of “blindly” applying FD

Outline

Review of Finite Difference Schemes

Application to the Diffusion Equation

1 – Review of Finite Difference Schemes

Finite differences

Finite difference schemes consist in replacing each derivative by a difference quotient.

Consider a function $u(x)$ of one variable.

Choose a *mesh size* Δx.

Approximate the value $u(j\Delta x)$ for $x = j\Delta x$ by a number u_j indexed by an integer j:

$$u_j \sim u(j\Delta x)$$

Approximations for the first derivative

The three standard approximations for the first derivative $\frac{\partial u}{\partial x}(j\Delta x)$ are

The backward difference: $\dfrac{u_j - u_{j-1}}{\Delta x}$

The centered difference: $\dfrac{u_{j+1} - u_{j-1}}{2\Delta x}$

The forward difference: $\dfrac{u_{j+1} - u_j}{\Delta x}$

Approximations for the first derivative

Each of them is a correct approximation, as shown by a Taylor expansion (assuming u is a C^4 function):

$$u(x+\Delta x) = u(x) + u'(x)\Delta x + \tfrac{1}{2}u''(x)(\Delta x)^2 + \tfrac{1}{6}u'''(x)(\Delta x)^3 + O(\Delta x)^4$$

Replacing Δx by $-\Delta x$, we get

$$u(x-\Delta x) = u(x) - u'(x)\Delta x + \tfrac{1}{2}u''(x)(\Delta x)^2 - \tfrac{1}{6}u'''(x)(\Delta x)^3 + O(\Delta x)^4$$

We deduce that

$$u'(x) = \frac{u(x) - u(x-\Delta x)}{\Delta x} + O(\Delta x)$$

$\Big\downarrow$ Taking $x = j\,\Delta x$

The backward difference: $\dfrac{u_j - u_{j-1}}{\Delta x}$

Approximations for the first derivative

Similarly for all three standard approximations:

$$u'(x) = \frac{u(x) - u(x - \Delta x)}{\Delta x} + O(\Delta x) \qquad \text{Backward difference}$$

$$= \frac{u(x + \Delta x) - u(x)}{\Delta x} + O(\Delta x) \qquad \text{Forward difference}$$

$$= \frac{u(x + \Delta x) - u(x - \Delta x)}{2\Delta x} + O(\Delta x)^2 \qquad \text{Centred difference}$$

Taking $x = j\Delta x$ we see that backward and forward differences are correct approximations to the order $O(\Delta x)$; and centered differences is a correct approximation to the order $O(\Delta x)^2$

Approximations for the second derivative

The simplest approximation for the second derivative is the

$$\text{centered second difference:} \quad u''(j\Delta x) \sim \frac{u_{j+1} - 2u_j + u_{j-1}}{(\Delta x)^2}$$

which is justified by the same Taylor expansions as used before, which when added give:

$$u''(x) = \frac{u(x+\ \Delta x) - 2u(x) + u(x - \Delta x)}{(\Delta x)^2} + O(\Delta x)^2$$

Centered second difference is thus valid with an error of $O(\Delta x)^2$

Functions of two variables

For a function of 2 variables $u(x,t)$, we choose a mesh size for both variables:

$$u(j\,\Delta x,\, n\,\Delta t) \sim u_j^n$$

The forward difference approximations of the first order partial derivatives are then for example

$$\frac{\partial u}{\partial t}(j\,\Delta x,\; n\,\Delta t) \sim \frac{u_j^{n+1} - u_j^n}{\Delta t} \qquad \frac{\partial u}{\partial x}(j\,\Delta x,\; n\,\Delta t) \sim \frac{u_{j+1}^n - u_j^n}{\Delta x}$$

Two types of errors are generally introduced in computations based on such approximations

① *Truncation errors* refers to the error introduced in the solutions by the approximations themselves, that is, the $O(\Delta x)$ terms

- local truncation error: on one term
- global truncation error: on the actual solution, combining all local contributions

② *Round off errors* occurs in a real computation because only a certain number of digits, typically 8 or 16, are retained by the computer at each step of the computation

2 – Application to the Diffusion Equation

Difference equation for Diffusion

Let us solve

$$u_t = u_{xx}, \qquad u(x,0) = \phi(x)$$

with a forward difference for u_t and a centered difference for u_{xx}.

We obtain the following difference equation:

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

The local truncation error is $O(\Delta t)$ for the left-hand side and $O(\Delta x)^2$ for the right-hand side.

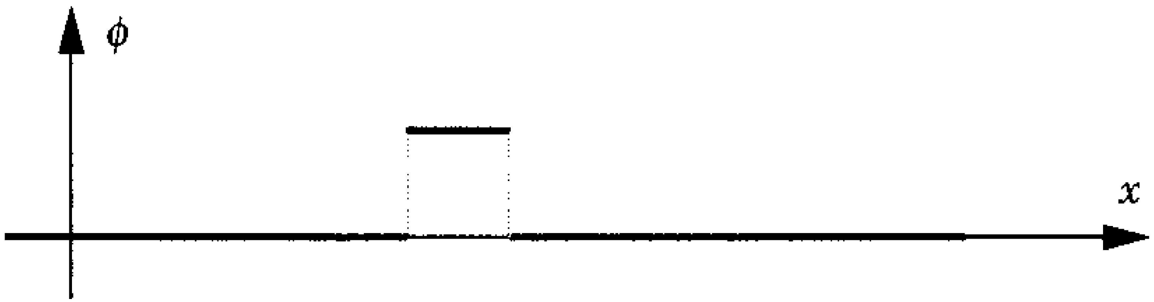
Difference equation for Diffusion

Let us choose a very small Δx and $\Delta t = (\Delta x)^2$.

This leads to the simplified equation:

$$u_j^{n+1} = u_{j+1}^n - u_j^n + u_{j-1}^n$$

Consider the following initial data $\phi(x)$



approximated by the following ϕ_j :

$$0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \qquad \rightarrow x$$

Difference equation for Diffusion

Applying the scheme we obtain:

$$
\begin{array}{l}
t \\
\uparrow
\end{array}
$$

$n=4$	1	-4	10	-16	19	-16	10	-4	1	
$n=3$	0	1	-3	6	-7	6	-3	1	0	
$n=2$	0	0	1	-2	3	-2	1	0	0	
$n=1$	0	0	0	1	-1	1	0	0	0	
$n=0$	0	0	0	0	1	0	0	0	0	$\rightarrow x$

This is *clearly* not correct: the initial data gets amplified and oscillates – which is not what we expect for diffusion.

We will analyze this in detail next week.

Take-home messages

- Finite difference approximations can be used to find approximate solutions to PDEs
- Small truncation errors do not guarantee that the solution will be close to the true solution

Next lecture

The diffusion equation:

1. Theory
2. Detailed stability analysis of FD approximation