

Lecture 1

Math 783

①

Text: Numerical Solution of Partial Differential Equations

by K.W. Morton and D.F. Mayers

Cambridge University Press, 1994

Scientific Computing

Physical motivation
Mathematical background
Numerical analysis techniques
Computer knowledge



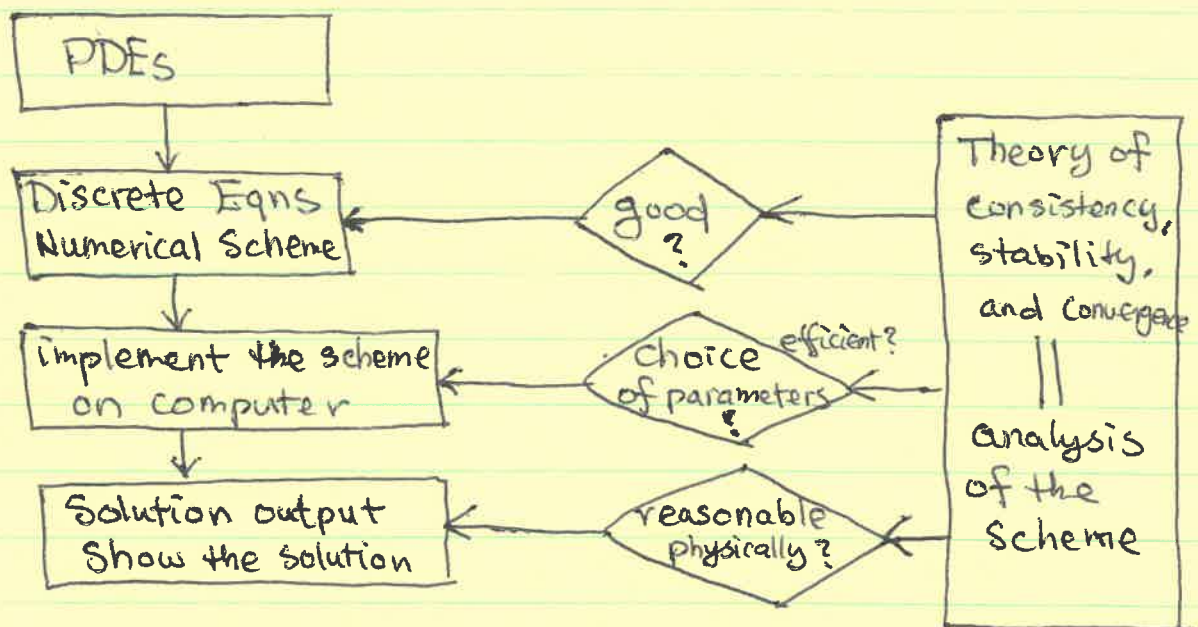
Find the numerical solution
of the practical problem



Show and illustrate your
numerical solution

(2)

Numerical Analysis or Computational Mathematics



Consistency : Does the numerical scheme or the discrete equation approach close enough to the original, continuous PDE ?

Stability : Does the numerical solution stay bounded during the course of the solution of the discrete equation ?

Convergence : Does the numerical solution of the discrete equation approach close enough to the exact solution (often is unknown) of the underlying Continuous PDE ?

About this course

	<u>Math 783</u>	<u>Math 796 (Fall, 96)</u>
<u>PDEs</u>	linear parabolic, hyperbolic, elliptic (mainly)	nonlinear, higher dimensions
<u>schemes</u>	basic	advanced
<u>discretization</u>	FD + FE	spectral
<u>Solution method</u>	basic, simple iteration	multigrid, preconditioning technique, conjugate gradient

Computer Knowledge:

C and/or Fortran 77 desired

Rounding error:

Four types of data:

integer 1, 0, -1, ...
 real = single, double 1.000000 14~16 digits
 logical = 'true' (1), 'false' (0)
 character 'hi', 'you'

Let us assume single precision (7 digits)

real number $1/3$ 0.333333 (computer expression)

$$\text{difference} = \frac{1}{3} - 0.333333 = 0.000000333 \dots$$

$$1.0 \quad 1.000001 \quad \text{or } 0.999999$$

$x, \tilde{x}$ (computer expression)

$$\text{Let } x = \tilde{x} + \varepsilon_x, y = \tilde{y} + \varepsilon_y, \varepsilon_x \approx 10^{-7}, \varepsilon_y \approx 10^{-7}$$

$$x \pm y \approx \tilde{x} \pm \tilde{y} = x \pm y - (\varepsilon_x \pm \varepsilon_y) \approx x \pm y \pm 2 \times 10^{-7}$$

$$x \cdot y : \tilde{x} \cdot \tilde{y} = x \cdot y + x \cdot \varepsilon_y + y \cdot \varepsilon_x \approx xy + (x+y) \times 10^{-7}$$

(4)

$$\begin{aligned}
\frac{x}{y} : \quad \frac{\tilde{x}}{\tilde{y}} &= \frac{x - \varepsilon_x}{y - \varepsilon_y} = \frac{1}{y} \cdot \frac{x - \varepsilon_x}{1 - \varepsilon_y/y} \\
&\approx \frac{1}{y} \cdot (x - \varepsilon_x) \left(1 + \varepsilon_y/y\right) \\
&= \frac{x}{y} - \frac{\varepsilon_x}{y} + \frac{x}{y} \cdot \frac{\varepsilon_y}{y} + o(\varepsilon_x \varepsilon_y) \\
&= \frac{x}{y} + \frac{10^{-7}}{|y|} + \frac{|x|}{|y|} \cdot \frac{10^{-7}}{|y|} \quad ? \text{ when } |y| \approx 0?
\end{aligned}$$

Conclusion: avoid the situation of y being small when compute $\frac{x}{y}$.

Chapter 2 Parabolic Equations in One Space Variable

§§ 2.1-2.4 An Explicit Scheme for the Model Problem

Linear parabolic equation

$$\text{PDE: } e(x,t) \frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left(a(x,t) \frac{\partial u}{\partial x} \right) + b(x,t) \frac{\partial u}{\partial x} + c(x,t)u + d(x,t)$$

where e and $a > 0$. IBVP:

$$\text{IC: } u(x,0) = u^0(x)$$

$$\text{BC: at } x=0, \quad \alpha_0(t)u + \alpha_1(t) \frac{\partial u}{\partial x} = \alpha_2(t) \\ (\alpha_0 \geq 0, \alpha_1 \leq 0, \alpha_0 - \alpha_1 > 0)$$

$$\text{at } x=1 \quad \beta_0(t)u + \beta_1(t) \frac{\partial u}{\partial x} = \beta_2(t) \\ (\beta_0 \geq 0, \beta_1 \geq 0, \beta_0 + \beta_1 > 0)$$

Analytical Method: Separation of variables

⊕ Fourier series expansion

Model Problem: IBVP

$$\begin{cases} u_t = u_{xx} & t_F > t > 0, \quad 0 < x < 1 \\ u(0,t) = u(1,t) = 0 & t_F > t > 0 \\ u(x,0) = u^0(x) & 0 < x < 1 \end{cases}$$

$$\begin{cases} u(x,t) = \sum_{m=1}^{\infty} a_m e^{-(m\pi)^2 t} \sin(m\pi x) \\ a_m = 2 \int_0^1 u^0(x) \sin(m\pi x) dx \end{cases}$$

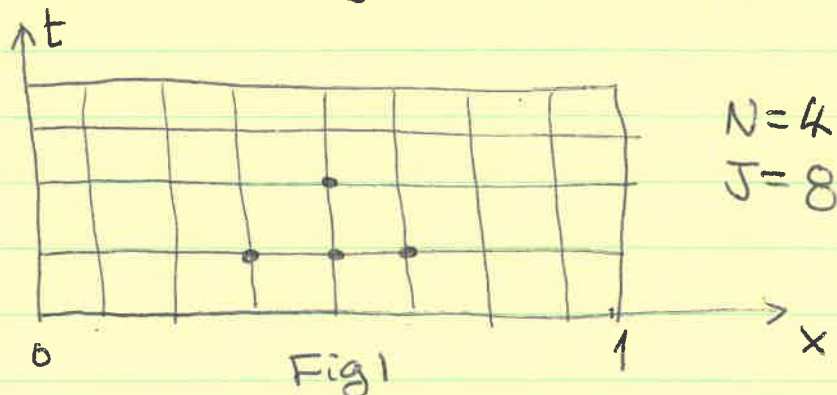
⑥

Mesh (Grid):

Spatial domain $x \in [0, 1]$, $\Delta x = \frac{1}{J}$, $x_j = j \Delta x$

time domain $t \in [0, t_F]$ $\Delta t = \frac{1}{N}$, $t_n = n \Delta t$

mesh points (x_j, t_n) $j=0, 1, \dots, J$, $n=0, 1, \dots, N$



objective a. Seek approximations of the solution at the mesh points

$$U_j^n \approx u(x_j, t_n)$$

b. $n=0$, $U_j^0 = u^0(x_j)$, $j=0, \dots, J$ (known)

c. $U_0^n = 0$, $U_J^n = 0$, $n=1, \dots, N$ (known)

d. $U_j^n = ?$ $j=1, 2, \dots, J-1$, $n=1, 2, \dots, N$

FD Discretization

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \quad 0 < x < 1, \quad 0 < t < t_F$$

$$\frac{\partial u}{\partial t}(x, t) = \frac{\partial^2 u}{\partial x^2}(x, t) \quad \text{for } 0 < x < 1, \quad 0 < t < t_F$$

$$\frac{\partial u}{\partial t}(x_j, t_n) = \frac{\partial^2 u}{\partial x^2}(x_j, t_n), \quad j=1, 2, \dots, J-1, \quad n=1, 2, \dots, N-1$$

From Calculus,

$$\lim_{\varepsilon \rightarrow 0} \frac{u(x_j, t_n + \varepsilon) - u(x_j, t_n)}{\varepsilon} = \frac{\partial u}{\partial t}(x_j, t_n)$$

$$\frac{u(x_j, t_n + \Delta t) - u(x_j, t_n)}{\Delta t} \approx \frac{\partial u}{\partial t}(x_j, t_n) \quad \text{if } \Delta t \text{ small}$$

(7)

$$\frac{u(x_{j+1}, t_n) - 2u(x_j, t_n) + u(x_{j-1}, t_n))}{(\Delta x)^2} \approx \frac{\partial^2 u}{\partial x^2}(x_j, t_n) \text{ if } \Delta x \ll 1$$

$$\frac{\partial u}{\partial t}(x_j, t_n) = \frac{\partial^2 u}{\partial x^2}(x_j, t_n) \implies$$

$$\frac{u(x_j, t_{n+1}) - u(x_j, t_n)}{\Delta t} \approx \frac{u(x_{j+1}, t_n) - 2u(x_j, t_n) + u(x_{j-1}, t_n))}{(\Delta x)^2}$$

Replacing $u(x_j, t_n)$ by U_j^n :

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

or

$$\boxed{U_j^{n+1} = U_j^n + \nu [U_{j+1}^n - 2U_j^n + U_{j-1}^n]} \quad (\text{Ex Sch})$$

$$\nu = \frac{\Delta t}{\Delta x^2}$$

Procedure: $U_j^n = ? \quad j=1, 2, \dots, J-1, n=1, 2, \dots, N$

① $n=0, U_j^0, j=0, 1, \dots, J$ known

Ex Sch $\implies U_j^1, j=1, 2, \dots, J-1$ } $n=1$ known
(r.h.s. known)
BCs $\implies U_0^1, U_J^1$

(See Fig 1)

② $n=1, U_j^1, j=0, 1, \dots, J$ known

Ex Sch $\implies U_j^2, j=1, 2, \dots, J-1$ } $n=2$ known
(r.h.s. known)
BCs $\implies U_0^2, U_J^2$

$\vdots$

Explicit