Numerical Methods for PDEs

A Finite Difference Scheme for the Heat Equation

(Lecture 3, Week 1)

Markus Schmuck

Department of Mathematics and Maxwell Institute for Mathematical Sciences Heriot-Watt University, Edinburgh

Edinburgh, 15 January, 2015











2/11

M. Schmuck (Heriot-Watt University) Numerical Methods for PDEs, Lecture 3

Goal: Find a suitable approximation w_j^n of the exact solution $u(x_j, t_n) = u_j^n$ at the mesh points (nodes) (x_j, t_n) of the dimensionless equation

$$u_t - u_{xx} = 0 \qquad x \in (0, 1), u(x, 0) = F(x), \quad t = 0, u(0, t) = \alpha(t), \quad t > 0, u(1, t) = \beta(t), \quad t > 0.$$

The simplest discrete approximation is the solution w_i^n of

 $D_t^+ w_j^n = D_x^2 w_j^n \,,$

at all interior points (x_j, t_n) , 0 < j < J, n > 0. **Remark.** *Note that*

 $u_t(x_j, t_n) \approx D_t^+ u_j^n, \qquad u_{xx}(x_j, t_n) \approx D_x^2 u_j^n$

and hence $D_t^+ u_j^n pprox D_x^2 u_j^n$.

M. Schmuck (Heriot-Watt University)

Numerical Methods for PDEs, Lecture 3



Goal: Find a suitable approximation w_j^n of the exact solution $u(x_j, t_n) = u_j^n$ at the mesh points (nodes) (x_j, t_n) of the dimensionless equation

$$u_t - u_{xx} = 0 \qquad x \in (0, 1), u(x, 0) = F(x), \quad t = 0, u(0, t) = \alpha(t), \quad t > 0, u(1, t) = \beta(t), \quad t > 0.$$

The simplest discrete approximation is the solution w_i^n of

 $D_t^+ w_j^n = D_x^2 w_j^n,$

at all interior points (x_j, t_n) , 0 < j < J, n > 0. Remark. Note that

 $u_t(x_j, t_n) \approx D_t^+ u_j^n, \qquad u_{xx}(x_j, t_n) \approx D_X^2 u_j^n$



Goal: Find a suitable approximation w_j^n of the exact solution $u(x_j, t_n) = u_j^n$ at the mesh points (nodes) (x_j, t_n) of the dimensionless equation

$$u_t - u_{xx} = 0 \qquad x \in (0, 1), u(x, 0) = F(x), \quad t = 0, u(0, t) = \alpha(t), \quad t > 0, u(1, t) = \beta(t), \quad t > 0.$$

The simplest discrete approximation is the solution w_i^n of

 $D_t^+ w_j^n = D_x^2 w_j^n \,,$

at all interior points (x_j, t_n) , 0 < j < J, n > 0. **Remark.** *Note that*

 $u_t(x_j,t_n) \approx D_t^+ u_j^n, \qquad u_{xx}(x_j,t_n) \approx D_x^2 u_j^n,$

Goal: Find a suitable approximation w_j^n of the exact solution $u(x_j, t_n) = u_j^n$ at the mesh points (nodes) (x_j, t_n) of the dimensionless equation

$$u_t - u_{xx} = 0 \qquad x \in (0, 1), u(x, 0) = F(x), \quad t = 0, u(0, t) = \alpha(t), \quad t > 0, u(1, t) = \beta(t), \quad t > 0.$$

The simplest discrete approximation is the solution w_i^n of

 $D_t^+ w_j^n = D_x^2 w_j^n,$

at all interior points (x_j, t_n) , 0 < j < J, n > 0. **Remark.** *Note that*

 $u_t(x_j,t_n) \approx D_t^+ u_j^n, \qquad u_{xx}(x_j,t_n) \approx D_X^2 u_j^n,$

and hence $D_t^+ u_j^n \approx D_x^2 u_j^n$.



The numerical scheme for w_i^n is explicit, that is,



Figure: Explicit finite difference scheme.

and after defining $r := \frac{k}{\hbar^2}$ and re-arranging, we get the

FTCS scheme: $w_j^{n+1} = rw_{j-1}^n + (1-2r)w_j^n + rw_{j+1}^n$.

FTCS = "Forward Time, Central Space"

M. Schmuck (Heriot-Watt University)

Numerical Methods for PDEs, Lecture 3



The numerical scheme for w_i^n is explicit, that is,



M. Schmuck (Heriot-Watt University)

Numerical Methods for PDEs, Lecture 3



The numerical scheme for w_i^n is explicit, that is,



Figure: Explicit finite difference scheme.

and after defining $r := \frac{k}{h^2}$ and re-arranging, we get the

FTCS scheme: $w_j^{n+1} = rw_{j-1}^n + (1 - 2r)w_j^n + rw_{j+1}^n$. (FTCS = "Forward Time, Central Space")



Algorithm:

- 1. Choose *J* and *r*; then calculate h = 1/J and $k = rh^2$.
- 2. Calculate (initial condition) $w_i^0 = F(x_i)$ and set n = 0.
- 3. Compute (explicit scheme)

$$w_j^{n+1} = rw_{j-1}^n + (1-2r)w_j^n + rw_{j+1}^n$$

for $j = 1, \ldots, J - 1$ and set (the boundary conditions)

$$w_0^{n+1} = \alpha(t_{n+1})$$
 and $w_J^{n+1} = \beta(t_{n+1})$.



Algorithm:

- 1. Choose J and r; then calculate h = 1/J and $k = rh^2$.
- 2. Calculate (initial condition) $w_i^0 = F(x_i)$ and set n = 0.
- 3. Compute (explicit scheme)

 $w_j^{n+1} = rw_{j-1}^n + (1-2r)w_j^n + rw_{j+1}^n$

for $j = 1, \ldots, J - 1$ and set (the boundary conditions)

 $w_0^{n+1} = \alpha(t_{n+1})$ and $w_J^{n+1} = \beta(t_{n+1})$.



Algorithm:

- 1. Choose J and r; then calculate h = 1/J and $k = rh^2$.
- 2. Calculate (initial condition) $w_i^0 = F(x_i)$ and set n = 0.
- 3. Compute (explicit scheme)

$$w_j^{n+1} = rw_{j-1}^n + (1-2r)w_j^n + rw_{j+1}^n$$

for $j = 1, \ldots, J - 1$ and set (the boundary conditions)

$$w_0^{n+1} = \alpha(t_{n+1})$$
 and $w_J^{n+1} = \beta(t_{n+1})$.



Algorithm:

- 1. Choose J and r; then calculate h = 1/J and $k = rh^2$.
- 2. Calculate (initial condition) $w_i^0 = F(x_i)$ and set n = 0.
- 3. Compute (explicit scheme)

$$w_j^{n+1} = rw_{j-1}^n + (1-2r)w_j^n + rw_{j+1}^n$$

for $j = 1, \ldots, J - 1$ and set (the boundary conditions)

$$w_0^{n+1} = \alpha(t_{n+1})$$
 and $w_J^{n+1} = \beta(t_{n+1})$.





Algorithm:

- 1. Choose J and r; then calculate h = 1/J and $k = rh^2$.
- 2. Calculate (initial condition) $w_i^0 = F(x_i)$ and set n = 0.
- 3. Compute (explicit scheme)

$$w_j^{n+1} = rw_{j-1}^n + (1-2r)w_j^n + rw_{j+1}^n$$

for $j = 1, \ldots, J - 1$ and set (the boundary conditions)

$$w_0^{n+1} = \alpha(t_{n+1})$$
 and $w_J^{n+1} = \beta(t_{n+1})$.





For the BCs $\alpha(t) = \beta(t) = 0$ and the IC $F(x) = \sin(\pi x)$ approximate the solution *u* of

$$\begin{cases} u_t - u_{xx} = 0 & x \in (0, 1), \\ u(x, 0) = F(x), & t = 0, \\ u(0, t) = \alpha(t), & t > 0, \\ u(1, t) = \beta(t), t > 0, \end{cases}$$

by the FTCS scheme with r = 0.4, J = 2 and two time steps.

The FTCS scheme: Use the Algorithm

- 1. J = 2, h = 1/J = 1/2, and $k = rh^2 = 0.4 \cdot 1/4 = 0.1$.
- 2. $w_j^0 = F(x_j) = \sin(\pi x_j)$ for $x_j = 0, 0.5, 1$, i.e.,

 $w_0^0 = \sin(0) = 0$, $w_1^0 = \sin(\pi/2) = 1$, and $w_2^0 = \sin(\pi) = 0$. Set n = 0.

- 3. Compute $w_1^1 = 0.4w_0^0 + (1 0.8)w_1^0 + 0.4w_2^0 = 0.2$ and set $w_0^1 = \alpha(t_1) = 0$ and $w_2^1 = \beta(t_1) = 0$.
- 4. Set n = 1 and repeat Step 3; $w_1^2 = 0.4w_0^1 + (1 - 0.8)w_1^1 + 0.4w_2^1 = 0 + 0.2 \cdot 0.2 + 0 = 0.$



For the BCs $\alpha(t) = \beta(t) = 0$ and the IC $F(x) = \sin(\pi x)$ approximate the solution *u* of

$$\begin{cases} u_t - u_{xx} = 0 & x \in (0, 1), \\ u(x, 0) = F(x), & t = 0, \\ u(0, t) = \alpha(t), & t > 0, \\ u(1, t) = \beta(t), t > 0, \end{cases}$$

by the FTCS scheme with r = 0.4, J = 2 and two time steps.

The FTCS scheme: Use the Algorithm

- 1. J = 2, h = 1/J = 1/2, and $k = rh^2 = 0.4 \cdot 1/4 = 0.1$.
- 2. $w_j^0 = F(x_j) = \sin(\pi x_j)$ for $x_j = 0, 0.5, 1$, i.e., $w_0^0 = \sin(0) = 0, w_1^0 = \sin(\pi/2) = 1$, and $w_2^0 = \sin(\pi) = 0$. Set n = 0.
- 3. Compute $w_1^1 = 0.4w_0^0 + (1 0.8)w_1^0 + 0.4w_2^0 = 0.2$ and set $w_0^1 = \alpha(t_1) = 0$ and $w_2^1 = \beta(t_1) = 0$.
- 4. Set n = 1 and repeat Step 3; $w_1^2 = 0.4w_0^1 + (1 - 0.8)w_1^1 + 0.4w_2^1 = 0 + 0.2 \cdot 0.2 + 0 = 0$



For the BCs $\alpha(t) = \beta(t) = 0$ and the IC $F(x) = \sin(\pi x)$ approximate the solution *u* of

$$\begin{cases} u_t - u_{xx} = 0 & x \in (0, 1), \\ u(x, 0) = F(x), & t = 0, \\ u(0, t) = \alpha(t), & t > 0, \\ u(1, t) = \beta(t), t > 0, \end{cases}$$

by the FTCS scheme with r = 0.4, J = 2 and two time steps.

The FTCS scheme: Use the Algorithm

- 1. J = 2, h = 1/J = 1/2, and $k = rh^2 = 0.4 \cdot 1/4 = 0.1$.
- 2. $w_j^0 = F(x_j) = \sin(\pi x_j)$ for $x_j = 0, 0.5, 1, i.e.,$
 - $w_0^0 = \sin(0) = 0$, $w_1^0 = \sin(\pi/2) = 1$, and $w_2^0 = \sin(\pi) = 0$. Set n = 0.
- 3. Compute $w_1^1 = 0.4w_0^0 + (1 0.8)w_1^0 + 0.4w_2^0 = 0.2$ and set $w_0^1 = \alpha(t_1) = 0$ and $w_2^1 = \beta(t_1) = 0$.
- 4. Set n = 1 and repeat Step 3;

 $w_1^2 = 0.4w_0^1 + (1 - 0.8)w_1^1 + 0.4w_2^1 = 0 + 0.2 \cdot 0.2 + 0 = 0.04$



For the BCs $\alpha(t) = \beta(t) = 0$ and the IC $F(x) = \sin(\pi x)$ approximate the solution *u* of

$$\begin{cases} u_t - u_{xx} = 0 & x \in (0, 1), \\ u(x, 0) = F(x), & t = 0, \\ u(0, t) = \alpha(t), & t > 0, \\ \end{cases} \quad u(1, t) = \beta(t), t > 0, \end{cases}$$

by the FTCS scheme with r = 0.4, J = 2 and two time steps.

The FTCS scheme: Use the Algorithm

- 1. J = 2, h = 1/J = 1/2, and $k = rh^2 = 0.4 \cdot 1/4 = 0.1$.
- 2. $w_j^0 = F(x_j) = \sin(\pi x_j)$ for $x_j = 0, 0.5, 1$, i.e., $w_0^0 = \sin(0) = 0, w_1^0 = \sin(\pi/2) = 1$, and $w_2^0 = \sin(\pi) = 0$. Set n = 0.
- Compute w₁¹ = 0.4w₀⁰ + (1 0.8)w₁⁰ + 0.4w₂⁰ = 0.2 and set w₀¹ = α(t₁) = 0 and w₂¹ = β(t₁) = 0.
 Set n = 1 and repeat Step 3; w₁² = 0.4w₀¹ + (1 0.8)w₁¹ + 0.4w₂¹ = 0 + 0.2 · 0.2 + 0 = 0.0

For the BCs $\alpha(t) = \beta(t) = 0$ and the IC $F(x) = \sin(\pi x)$ approximate the solution *u* of

$$\begin{cases} u_t - u_{xx} = 0 & x \in (0, 1), \\ u(x, 0) = F(x), & t = 0, \\ u(0, t) = \alpha(t), & t > 0, \\ \end{cases} \quad u(1, t) = \beta(t), t > 0, \end{cases}$$

by the FTCS scheme with r = 0.4, J = 2 and two time steps.

The FTCS scheme: Use the Algorithm

- 1. J = 2, h = 1/J = 1/2, and $k = rh^2 = 0.4 \cdot 1/4 = 0.1$.
- 2. $w_j^0 = F(x_j) = \sin(\pi x_j)$ for $x_j = 0, 0.5, 1$, i.e., $w_0^0 = \sin(0) = 0, w_1^0 = \sin(\pi/2) = 1$, and $w_2^0 = \sin(\pi) = 0$. Set n = 0.
- 3. Compute $w_1^1 = 0.4w_0^0 + (1 0.8)w_1^0 + 0.4w_2^0 = 0.2$ and set $w_0^1 = \alpha(t_1) = 0$ and $w_2^1 = \beta(t_1) = 0$.
- 4. Set n = 1 and repeat Step 3; $w_1^2 = 0.4w_0^1 + (1 - 0.8)w_1^1 + 0.4w_2^1 = 0 + 0.2 \cdot 0.2 + 0 = 0.04$



We only needed to compute the solution at the points • in the figure below, i.e., for t = 0.1, 0.2 with values $w_1^1 = 0.2$ and $w_1^2 = 0.04$.



Exercises :

1. Is there a general solution w_1^n in the above example? 2. Repeat the above steps for J = 3.

M. Schmuck (Heriot-Watt University)

Numerical Methods for PDEs, Lecture 3



We only needed to compute the solution at the points • in the figure below, i.e., for t = 0.1, 0.2 with values $w_1^1 = 0.2$ and $w_1^2 = 0.04$.



Exercises :

- 1. Is there a general solution w_1^n in the above example?
- 2. Repeat the above steps for J = 3.



Example 2: "Triangular" initial conditions

Repeating Example 1 with J = 4 and the "triangular" initial condition

$${\cal F}(x) = egin{cases} 2x, & x \leq 0.5 \ 2(1-x), & x > 0.5 \end{cases},$$

leads to problems (due to the discontinuous derivative), see Figure below.



Example 2: "Triangular" initial conditions

Repeating Example 1 with J = 4 and the "triangular" initial condition

$$F(x) = egin{cases} 2x, & x \leq 0.5 \ 2(1-x), & x > 0.5 \end{cases},$$

leads to problems (due to the discontinuous derivative), see Figure below.



Figure: Left: r = 0.4, w_j^n slowly decreases to zero (as expected). Right: r = 0.6, w_i^n shows spatial oscillations.

M. Schmuck (Heriot-Watt University)

Numerical Methods for PDEs, Lecture 3



- 1. Already for small (times) t_n , the temperature w_j^n becomes negative.
- 2. Spatial oscillations become unbounded

 $w^n_j o \infty$ for $n o \infty$

in contrast to the exact solution

 $u \to 0$ for $t \to \infty$.

A numerical scheme with this sort of bad behavior (e.g. nonphysical/unbounded oscillations) is called *unstable*.

We study ways of analysing this behaviour over the next few lectures.



- 1. Already for small (times) t_n , the temperature w_j^n becomes negative.
- 2. Spatial oscillations become unbounded

$$w_j^n \to \infty$$
 for $n \to \infty$

in contrast to the exact solution

$$u \to 0$$
 for $t \to \infty$.

A numerical scheme with this sort of bad behavior (e.g. nonphysical/unbounded oscillations) is called *unstable*.

We study ways of analysing this behaviour over the next few lectures.



- 1. Already for small (times) t_n , the temperature w_j^n becomes negative.
- 2. Spatial oscillations become unbounded

$$w_i^n \to \infty$$
 for $n \to \infty$

in contrast to the exact solution

$$u \to 0$$
 for $t \to \infty$.

A numerical scheme with this sort of bad behavior (e.g. nonphysical/unbounded oscillations) is called *unstable*.

We study ways of analysing this behaviour over the next few lectures.



- 1. Already for small (times) t_n , the temperature w_j^n becomes negative.
- 2. Spatial oscillations become unbounded

$$w_j^n \to \infty$$
 for $n \to \infty$

in contrast to the exact solution

$$u \to 0$$
 for $t \to \infty$.

A numerical scheme with this sort of bad behavior (e.g. nonphysical/unbounded oscillations) is called *unstable*.

We study ways of analysing this behaviour over the next few lectures.



1. What does FTCS mean?

2. What is the FTCS scheme for the heat equation?

3. What are the characteristics of an unstable scheme?



11/11

M. Schmuck (Heriot-Watt University) Numerical Methods for PDEs, Lecture 3

1. What does FTCS mean?

2. What is the FTCS scheme for the heat equation?

3. What are the characteristics of an unstable scheme?



1. What does FTCS mean?

2. What is the FTCS scheme for the heat equation?

3. What are the characteristics of an unstable scheme?

