Numerical Methods for PDEs

Diffusion/Heat Conduction and Finite Differences

(Lecture 2, Week 1)

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Outline

Diffusion/Heat conduction

Consider the parabolic problem (diffusion/heat conduction)

$$\begin{cases} U_T - KU_{XX} = 0 & \text{on} \quad 0 < X < L\,,\ T > 0\,, \\ U(X,0) = U_0(X) & \text{on} \quad 0 < X < L\,, \\ U(0,T) = g_0(T)\,, & \\ U(1,T) = g_1(T)\,. & \end{cases}$$

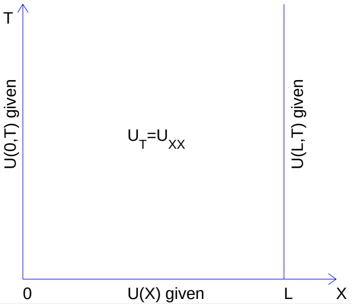

Figure: Heat conduction. Find solution $U(X,T)$ in open box $T > 0$, $X \in (0,L)$.

Different applications: Generally show different scales (e.g. length, time)

Introduce dimensionless variables:

$$x := \frac{X}{L}, \quad t := \frac{K}{L^2} T, \quad u := \frac{U}{\overline{U}},$$

where L, $\overline{U}$, and $\frac{K}{L^2}$ are a *characteristic length*, a *characteristic concentration/temperature*, and the *diffusion time*, respectively.

Herewith, we obtain the dimensionless equation

$$u_t - u_{xx} = 0, \text{ on } (0,1),\ t > 0,$$

which is generally the *"standard form"* of equations for numerical considerations.

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Notation and basic definitions

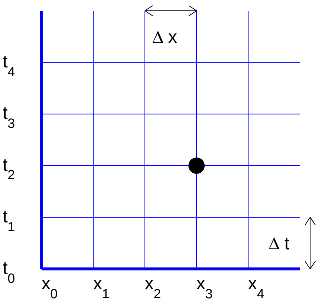

Figure: Finite difference mesh/grid Ω_h.

We introduce the following discretisation ($h = \Delta x$, $k = \Delta t$)

$$x_j = jh\,, \quad j = 0, 1, \dots, J\,, \quad h := 1/J$$
$$t_n = nk\,, \quad n = 0, 1, \dots, N\,, \quad k > 0\,,$$

which allows us to replace $\Omega = (0,1)$ and $\overline{\Omega} = (0,1)$ by a mesh/grid

$$\Omega_h := \{x_j\,,\, j = 1, \ldots, J-1\}\,, \quad \Gamma_h := \{x_0, x_J\} \quad \text{"boundary"}\,,$$
$$\overline{\Omega}_h := \{x_j\,,\, j = 0, 1, \ldots, J\}\,.$$

Defintion. *We denote the exact solution u at grid point (x_j, t_n) by $u_j^n := u(x_j, t_n)$ and w_j^n for its FD approximation.*

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Definition. *We define the following difference quotients*

$$\begin{cases} D_x^+ u_j^n := \frac{F_{x_j} u(x,t_n)}{h} := \frac{u_{j+1}^n - u_j^n}{h} & \textit{Forward Difference}\,, \\ D_x^- u_j^n := \frac{B_{x_j} u(x,t_n)}{h} := \frac{u_j^n - u_{j-1}^n}{h} & \textit{Backward Difference}\,, \\ D_x^0 u_j^n := \frac{D_{x_j} u(x,t_n)}{2h} := \frac{u_{j+1}^n - u_{j-1}^n}{2h} & \textit{Central Difference}\,, \\ D_x^2 u_j^n := \frac{\delta_{x_j}^2 u(x,t_n)}{h^2} := \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2} & \textit{Second Central Difference}\,, \end{cases}$$

It holds that

$$D_x^0 u_j^n = \frac{1}{2}\left(D_x^+ u_j^n + D_x^- u_j^n\right) \quad \text{and} \quad D_x^2 u_j^n = D_x^+ D_x^- u_j^n = D_x^- D_x^+ u_j^n\,,$$

and by Taylor's formula

$$\begin{cases} D_x^+ u_j^n = u_x(x_j,t_n) + \frac{h}{2} u_{xx}(x_j,t_n) + \mathcal{O}(h^2)\,, \\ D_x^- u_j^n = u_x(x_j,t_n) - \frac{h}{2} u_{xx}(x_j,t_n) + \mathcal{O}(h^2)\,, \\ D_x^0 u_j^n = u_x(x_j,t_n) + \mathcal{O}(h^2)\,, \\ D_x^2 u_j^n = u_{xx}(x_j,t_n) + \mathcal{O}(h^2)\,. \end{cases}$$

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Example

Claim:

$$D_x^+ D_t^+ u_j^n = \frac{F_{x_j} F_{t_n} u(x,t)}{hk} = u_{tx}(x_j, t_n) + \mathcal{O}(h,k)\,.$$

Proof:

$$\begin{aligned} D_x^+ D_t^+ u_j^n &= D_x^+ \left(\frac{u_j^{n+1} - u_j^n}{k} \right) \\ &= D_x^+ \left(u_t(x_j, t_n) + \frac{k}{2} u_{tt}(x_j, t_n) + \mathcal{O}(k^2) \right) \\ &= D_x^+ u_t(x_j, t_n) + \frac{k}{2} D_x^+ u_{tt}(x_j, t_n) + \mathcal{O}(k^2)\,, \end{aligned}$$

if u is regular/smooth enough.

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Proof:

$$\begin{aligned}
D_x^+ D_t^+ u_j^n &= D_x^+ \left(\frac{u_j^{n+1} - u_j^n}{k} \right) \\
&= D_x^+ \left(u_t(x_j, t_n) + \frac{k}{2} u_{tt}(x_j, t_n) + \mathcal{O}(k^2) \right) \\
&= D_x^+ u_t(x_j, t_n) + \frac{k}{2} D_x^+ u_{tt}(x_j, t_n) + \mathcal{O}(k^2)\,,
\end{aligned}$$

if u is regular/smooth enough.

Moreover,

$$D_x^+ u_t(x_j, t_n) = u_{tx}(x_j, t_n) + \frac{h}{2} u_{txx}(x_j, t_n) + \mathcal{O}(h^2)\,,$$
$$D_x^+ u_{tt}(x_j, t_n) = u_{ttx}(x_j, t_n) + \frac{h}{2} u_{ttxx}(x_j, t_n) + \mathcal{O}(h^2)\,,$$

and therefore

$$\begin{aligned} D_x^+ D_t^+ u_j^n &= \left\{ u_{tx}(x_j, t_n) + \frac{h}{2} u_{txx}(x_j, t_n) + \mathcal{O}(h^2) \right\} \\ &\quad + \frac{k}{2} \left\{ u_{ttx}(x_j, t_n) + \frac{h}{2} u_{ttxx}(x_j, t_n) + \mathcal{O}(h^2) \right\} + \mathcal{O}(k^2) \\ &= u_{tx}(x_j, t_n) + \mathcal{O}(h, k)\,. \end{aligned}$$

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Example: FD approximation in Maple

Define the function and calculate exact partial derivatives

```
> u:=(x,t)->exp(-t)*sin(x);
  dux:=diff(u(x,t),x);
  dut:=diff(u(x,t),t);
  duxx:=diff(u(x,t),x,x);
```

Result:

$$u := (x,t) \to e^{(-t)} \sin(x)$$

$$dux := e^{(-t)} \cos(x)$$

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Evaluate exact partial derivatives at given point

```
> p := x=0.5, t:=0.1;
  subs(p,dux); ex:=evalf(%);
  subs(p,dut); et:=evalf(%);
  subs(p,duxx); exx:=evalf(%);
```

Result:

$$p := x = 0.5, t := 0.1$$

$$e^{-.01}\cos(0.5)$$

$$ex := 0.7940695394$$

$$-e^{-0.1}\sin(0.5)$$

$$et := -.4338021665$$

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(Note that u satifies the heat equation $u_t = u_{xx}$)

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Forward difference approximation of *ux* and *ut*

```
> h:=0.1; k:=0.1;
> subs(p,(u(x+h,t)-u(x,t))/0.1);
  evalf(%); 'error' = ex-%;
  subs(p,(u(x,t+k)-u(x,t))/0.1);
  evalf(%); 'error' = et-%;
```

$$deltax = 0.1$$

$$10.e^{-.1}\cos(0.6) - 10.e^{-.1}\sin(0.5)$$

$$0.771074712$$

$$error = 0.0229948274$$

$$deltat := 0.1$$

$$10.e^{-0.2}\sin(0.5) - 10.e^{-0.1}\sin(0.5)$$

$$-.412817342$$

$$error = -0.0209848245$$

Central difference approximation of *ux* and *ut*

```
> subs(p,(u(x+h,t)-u(x-h,t))/0.2);
  evalf(%); 'error' = ex-%;
  subs(p,(u(x,t+k)-u(x,t-k))/0.2);
  evalf(%); 'error' = et-%;
```

$$5.e^{-.1}\cos(0.6) - 5.e^{-.1}\sin(0.4)$$

$$0.792746751$$

$$error = 0.0013227884$$

$$5.e^{-0.2}\sin(0.5) - 5.e^{0.}\sin(0.5)$$

$$-.434525531$$

$$error = 0.007233645$$

2nd central difference approximation of *uxx*

```
> subs(p,(u(x+h,t)-2u(x,t)+u(x-h,t))/0.1^2);
  evalf(%); 'error' = exx-%;
```

$$100.e^{-0.1}\cos(0.6) - 200.e^{-0.1}\sin(0.5) + 100.e^{-0.1}\sin(0.4)$$

$$0.43344079$$

$$error = 0.0003613765$$

Summary of learning targets:

1. Which PDE describes diffusion/heat conduction?
2. Which typical timescale allows us to bring the diffusion equation into a dimensionless form?
3. What are the four essential difference operators and how are they defined?

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