Model 1

$$\frac{\partial u}{\partial t} = \kappa \cdot \frac{\partial^2 u}{\partial x^2}$$

heat equation (diffusion equation)

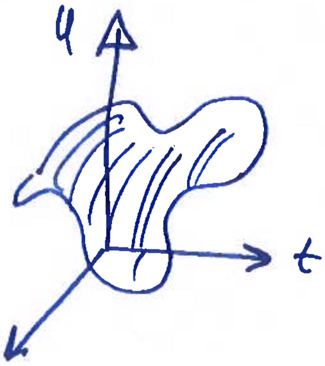
partial derivatives

P.D.E. — partial differential equation

$u(x,t) = ?$

temperature

$\kappa > 0$: conduction coefficient (diffusion " ")



space $x \in [0,1]$ — special case

time $t \in [0,T]$ — given (final time)

IC: $u(x,0) = u_0(x) = \sin(\pi x)$

initial condition — given — special case

BCs : $u(0,t) = 0$, $u(1,t) = 0$

boundary conditions — special case

theory

$\Rightarrow u(x,t) = e^{-\pi^2 t} \sin(\pi x)$

Numerical solutions with Matlab:

"Method-of-Lines" (two steps: first space x, then time t)

1) a) Δx Δx Δx ... (SPACE) x

$x_1 = 0$, x_2, x_3, x_4 ... $1 = x_I$ ← final index

a "uniform grid"

$$\boxed{\begin{array}{l} x_i = (i-1)\Delta x \\ i = 1,2,3,\dots,I \end{array}}$$

$x_1 = 0$, $x_2 = \Delta x$

... $x_I = (I-1)\Delta x$

(2

$\Rightarrow\ i = I:\ (I-1)\Delta x = x_I = 1$

$$\Rightarrow \boxed{\Delta x = \frac{1}{I-1}}$$

choose one of the two

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1 b) approximate $\frac{\partial^2 u}{\partial x^2}$ at $x = x_i$:

$$\frac{\partial^2 u}{\partial x^2}(x_i, t) \approx \frac{u_{i+1}(t) - 2u_i(t) + u_{i-1}(t)}{(\Delta x)^2}$$

follows from Taylor expansions (see: "Numerieke wiskunde" / numerical analysis course)

error: $\mathcal{O}((\Delta x)^2)$

with $u_i(t) \approx u(x_i, t)$

exact value at discrete x_i's and continuous t

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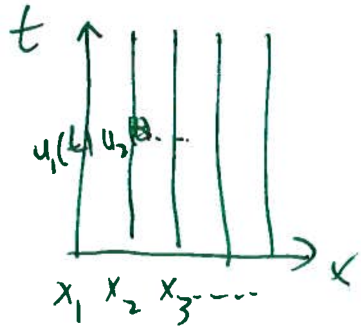
1 c) Define

$$\boxed{\vec{u}(t) \stackrel{\text{def}}{=} \begin{pmatrix} u_1(t) \\ u_2(t) \\ \vdots \\ u_{I-1}(t) \end{pmatrix}} \approx \begin{pmatrix} u(x_1,t) \\ u(x_2,t) \\ \vdots \\ u(x_{I-1},t) \end{pmatrix}$$



$$\Rightarrow \frac{\partial u}{\partial t}(x_i, t) \approx \frac{d}{dt}(u_i(t)) = \dot{u}_i(t)$$

$$\Longrightarrow \frac{d\vec{u}}{dt}(t) = \underbrace{\frac{1}{(\Delta x)^2}\begin{pmatrix} \ddots & & 0 \\ & 1\ -2\ 1 & \\ 0 & & \ddots \end{pmatrix}}_{\text{call matrix } D_2} \vec{u}(t)$$

(tri-diagonal with eigenvalues: $\lambda_i = \frac{-4}{(\Delta x)^2} \sin^2\left(\frac{\pi i \Delta x}{2}\right)$) $\underline{\underline{\in \mathbb{R}^-}}$

and more to the left for smaller Δx

$$\begin{cases} \dot{u}_1 = 0, & u_1(0) = \sin(\pi x_1) = \sin(0) = 0 \\ \dot{u}_2 = \frac{u_3 - 2u_2 + u_1}{(\Delta x)^2}, & u_2(0) = \sin(\pi x_2) \\ \dot{u}_3 = \frac{u_4 - 2u_3 + u_2}{(\Delta x)^2}, & u_3(0) = \sin(\pi x_3) \\ \vdots & \vdots \\ \dot{u}_{I-1} = \frac{u_I - 2u_{I-1} + u_{I-2}}{(\Delta x)^2}, & u_{I-1}(0) = \sin(\pi x_{I-1}) \\ \dot{u}_I = 0, & u_I(0) = \sin(\pi x_I) = \sin(\pi) = 0 \end{cases}$$

1d) BCs: $\begin{cases} u_0 = 0 \\ u_I = 0 \end{cases}$ $\rightsquigarrow$ can be used in the first row and last row of the matrix D_2

IC: $\vec{u}(0) = \begin{pmatrix} \sin(\pi x_1) \\ \sin(\pi x_2) \\ \vdots \\ \sin(\pi x_{I}) \end{pmatrix} \overset{\text{def}}{=} \vec{u}_0$

$\Rightarrow$ ODE system: $\begin{cases} \dot{\vec{u}}(t) = D_2 \vec{u}(t) \\ \vec{u}(0) = \vec{u}_0 \end{cases}$ known

ordinary

$\Downarrow$ solution

$$\vec{u}(t) = e^{tD_2} \vec{u}_0$$

in Matlab: "expm"

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2) Euler-Forward (Explicit Euler) note that matlab does not have zero-index $\to$ re-write starting from index 1

"EF"

explicit: $\dfrac{\vec{u}^{n+1} - \vec{u}^n}{\Delta t} = D_2 \vec{u}^n$ $\quad n = 0, 1, 2, \ldots, N$ ($\sim t=0$, $\sim t=T$)

time step.

time points: $t^n = (n-1)\Delta t$

$n = 1, \ldots, N$

$t^N = T = (N-1)\Delta t$

$$\vec{u}^{n+1} = (I + \Delta t D_2)\vec{u}^n$$

choose one of the two $\quad \boxed{\Delta t = \dfrac{T}{N-1}}$ given

or

Euler-Backward (implicit Euler)

"EB"

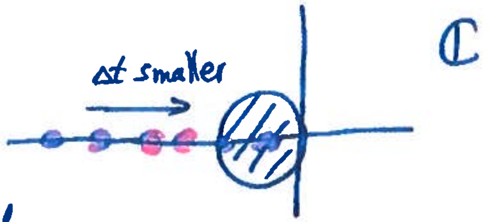
implicit: $\dfrac{\vec{u}^{n+1} - \vec{u}^n}{\Delta t} = D_2 \vec{u}^{n+1} \Rightarrow \underbrace{(I - \Delta t D_2)}_{A}\vec{u}^{n+1} = \vec{u}^n$

in Matlab: " $\vec{u}^{n+1} = A \backslash \vec{u}^n$ "

for loop in n-index

property of EF : numerically stable solutions, if $\frac{\Delta t}{(\Delta x)^2} \leq \frac{1}{2}$

$\Leftrightarrow$ eigenvalues of D_2 lie in a unit circle :



for higher resolution in space we need small Δx and, therefore, Δt "quadratically" smaller (expensive)

property of EB :

numerically stable solutions for all $\Delta t > 0$!

BUT, we need to solve a linear system to obtain $\vec{u}^{n+1}$ from $\vec{u}^{n}$

$\vec{u}^{n+1}$ at t^{n+1}, $\vec{u}^{n}$ at t^{n}

Note: the accuracy in space of EF ≈ EB

$\boxed{\text{Model 2}}$

$$\frac{\partial u}{\partial t} = d \cdot \frac{\partial^2 u}{\partial x^2} + \gamma \, \underbrace{u(1-u)}_{\text{nonlinear term}}, \quad d > 0$$

"Fisher PDE"

(population dynamics)

follow recipe in Model 1 :

$$\Rightarrow \quad \dot{\vec{u}}(t) = d\, D_2 \vec{u}(t) + \vec{f}(\vec{u}(t))$$

$$\vec{f}(\vec{u}(t)) = \begin{pmatrix} \gamma u_1(1-u_1) \\ \gamma u_2(1-u_2) \\ \vdots \\ \gamma u_{I-1}(1-u_{I-1}) \end{pmatrix}$$

(2) check what would happen, if EB is applied

(... ⇒ solve huge nonlinear system at each step $t^n \to t^{n+1}$)

(1) EF: $\frac{\vec{u}^{n+1} - \vec{u}^{n}}{\Delta t} = d\, D_2 \vec{u}^{n} + \vec{f}^{n} \Rightarrow \vec{u}^{n+1} = (I + d \Delta t D_2)\vec{u}^{n} + \Delta t \vec{f}^{n}$

loop in index n ($n \neq 0$!!)

find a "mix" between EF and EB:

not always stable (see heat equation) — EF

always stable but "expensive" — EB

$\rightsquigarrow$ IMEX method

IM: implicit (EB); EX: explicit (EF)

$$\Rightarrow \quad \frac{\vec{u}^{n+1} - \vec{u}^{n}}{\Delta t} = d\, D_2\, \vec{u}^{n+1} + \vec{f}(\vec{u}^{n})$$

$$\Rightarrow \quad \vec{u}^{n+1} - \vec{u}^{n} = d\,\Delta t\, D_2\, \vec{u}^{n+1} + \Delta t\, \vec{f}(\vec{u}^{n})$$

not to forget!

$$\Rightarrow \quad \underbrace{(I - d\,\Delta t\, D_2)}_{\text{known matrix, call: } A}\, \vec{u}^{n+1} = \underbrace{\vec{u}^{n} + \Delta t\, \vec{f}(\vec{u}^{n})}_{\text{known from previous step, call: } \vec{g}(\vec{u}^{n})}$$

$\vec{u}^{n+1}$: to be determined for $n = 0, 1, 2, \dots, N-1$

$$\Rightarrow \quad \boxed{A\, \vec{u}^{n+1} = \vec{g}(\vec{u}^{n})} \quad \text{a linear system}$$

" $\vec{u}^{n+1} = A \backslash \vec{g}^{n}$ "

Model 3

$$u_t = d u_{xx} + \left(\frac{u^2}{2}\right)_x + \tau u_{xxt} \quad \text{(from geohydrology)}$$

u_t: short notation for $\frac{\partial u}{\partial t}$

u_{xx}: $\frac{\partial^2 u}{\partial x^2}$

$(\ )_x$: $\frac{\partial}{\partial x}(\ )$

u_{xxt}: $\frac{\partial^3}{\partial x^2 \partial t}$

one-phase: "water"

non-monotone waves ("fingers")

$d > 0, \ \tau \geq 0$

two-phase: water - oil
or
water - oxygen
or
- -

$$\frac{u^2}{u^2 + M(1-u)^2}$$

$$M = \frac{\mu_w}{\mu_o}$$

viscosity

Method-of-lines ("M.o.L."):

$$\dot{\vec u}(t) = d\, D_2 \vec u(t) + \underbrace{\vec h(\vec u(t))}_{} + \tau D_2\, \dot{\vec u}(t)$$

$$\underbrace{(I - \tau D_2)}_{\substack{\text{call: } M \\ \text{(matrix)}}}\, \dot{\vec u}(t) = d D_2 \vec u(t) + \vec h(\vec u(t))$$

2 → IMEX

$$M\, \frac{\vec u^{\,n+1} - \vec u^{\,n}}{\Delta t} = d D_2 \vec u^{\,n+1} + \vec h(\vec u^{\,n})$$

$$\Rightarrow\ M(\vec u^{\,n+1} - \vec u^{\,n}) = d\,\Delta t\, D_2 \vec u^{\,n+1} + \Delta t\, \vec h(\vec u^{\,n})$$

$$\Rightarrow\ \underbrace{(M - d\,\Delta t\, D_2)}_{\substack{\text{call: } B \\ \text{(matrix)}}}\, \vec u^{\,n+1} = \underbrace{M \vec u^{\,n} + \Delta t\, \vec h(\vec u^{\,n})}_{\text{call: } \vec k(\vec u^{\,n})}$$

$$\Rightarrow\ \boxed{B \vec u^{\,n+1} = \vec k(\vec u^{\,n})} \ \rightarrow\ \vec u^{\,n+1} = B \backslash \vec k^{\,n}$$

at $x = x_i$: $\left(\frac{u^2}{2}\right)_x \approx \frac{u_{i+1}^2 - u_{i-1}^2}{4\Delta x}$

(Comes from: $u_x \approx \frac{u_{i+1} - u_{i-1}}{2\Delta x}$

Taylor (num. analysis) central finite differences

$$\vec h(\vec u(t)) = \begin{pmatrix} \frac{u_2^2 - u_0^2}{4\Delta x} \\ \frac{u_3^2 - u_1^2}{4\Delta x} \\ \vdots \end{pmatrix} \quad u_0 = 0$$

check final term

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1 EF:

$$\frac{\vec u^{\,n+1} - \vec u^{\,n}}{\Delta t} = d D_2 \vec u^{\,n} + \vec h^{\,n} + \tau D_2 \frac{\vec u^{\,n+1} - \vec u^{\,n}}{\Delta t}$$

$$\underbrace{(I - \tau D_2)}_{=M}\, \vec u^{\,n+1} = \underbrace{(I + d\,\Delta t\, D_2 - \tau D_2)}_{=B}\, \vec u^{\,n}$$

$\vec u^{\,n+1} = M \backslash (B \vec u^{\,n})$ loop in index n