Műegyetem 1782

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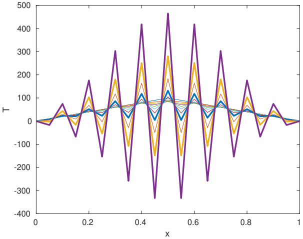
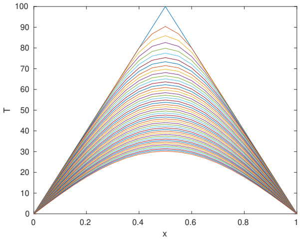
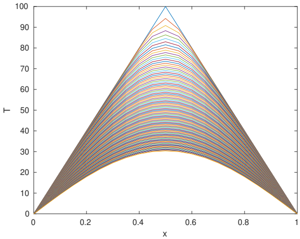
NES Laboratórium

MűFi23

Parabolic PDEs - Finite Difference Solution







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Reichardt András | (2023. november 5.)

Example of parabolic type PDE

- Heat conduction problem - start at 1D unsteady heat-diffusion in a solid

$$\dot{q} = -k \cdot A \cdot \frac{dT}{dn}$$

$$\dot{q}_{net,x} = \dot{q}(x) - \dot{q}(x + dx) = \dot{q}(x) - \left[\dot{q}(x) + \frac{\partial \dot{q}(x)}{\partial x} \mathrm{dx}\right] = -\frac{\partial \dot{q}(x)}{\partial x}$$

$$\dot{q}_{net,x} = -\frac{\partial}{\partial x}\left(-kA\frac{\partial T}{\partial x}\right) dx = \frac{\partial}{\partial x}\left(k \cdot \frac{\partial T}{\partial x}\right) dV$$

$$\dot{q}_{net,y} = \frac{\partial}{\partial y}\left(k \cdot \frac{\partial T}{\partial y}\right) dV; \qquad \dot{q}_{net,z} = \frac{\partial}{\partial z}\left(k \cdot \frac{\partial T}{\partial z}\right) dV$$

- $$\dot{q}_{net} = \dot{q}_{net,x} + \dot{q}_{net,y} + \dot{q}_{net,z}$$
- in steady state - no net change in the amount of the energy stored in the solid
$$\int_V \dot{q}_{net} dV = 0$$
$$\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(k\frac{\partial T}{\partial x}\right) = 0$$
- in nabla notation
$$\nabla\left(k\nabla T\right) = 0$$
- if k is constant in t and x
$$\nabla^2 T = 0$$

this is an elliptic PDE!

- steady state heat equation with internal energy generation ($\dot{E}$ - J/s)

$$\dot{E} = \dot{Q}(x, y, z) \cdot dV$$

  where $\dot{Q}$ is energy generation rate per unit volume

- steady heat flow - sum of energy transferred to the solid and internal generation (or loss) must equal zero

$$\partial_x(k\partial_x T) + \partial_y(k\partial_y T) + \partial_z(k\partial_z T) + \dot{Q} = 0$$

- $$\nabla\left(k\nabla T\right) = \dot{Q}$$

  or in case of constant k

$$\nabla^2 T = -\frac{\dot{Q}}{k}$$

Unsteady heat diffusion problem

- energy (E, [J]) stored in the solid, mass dm [kg]

$$E_{stored} = dm \cdot C \cdot T = (\varrho \cdot dV) \cdot C \cdot T = \varrho \cdot C \cdot T \cdot dV$$

$$\frac{\partial E_{stored}}{\partial t} = \nabla \left(k \nabla T \right) + \dot{Q}$$

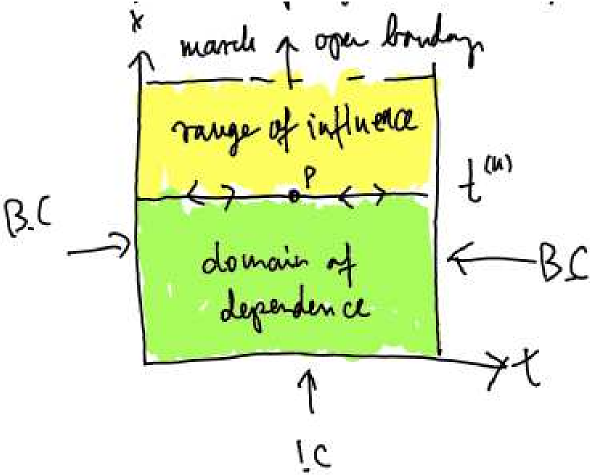
- constant material parameters :

$$\frac{\partial (\varrho C T)}{\partial t} = \varrho \cdot C \cdot \frac{\partial T}{\partial t}$$

- $$\frac{\partial T}{\partial t} = \nabla \left(\frac{k}{\varrho C} \cdot \nabla T \right) + \frac{\dot{Q}}{\varrho C}$$

- unsteady heat diffusion problem is a propagation problem, which must be solved by marching methods

- propagation problem is an initial-boundary-value problem in open domain $D(x, t)$
- infinity physical information propagation speed
- point P at time t^n influences the solution at all other points "above"
- solution at P on t^n depends on all points "under" it



- $$f_t = \alpha \cdot f_{xx}, \qquad f(x,0) = \phi(x) = A_m \cdot e^{jk_m x}$$
- exact solution :

$$f(x,t) = e^{-\alpha \cdot k_m^2 t} \cdot \phi(x) = e^{-\alpha \cdot k_m^2 t} \cdot A_m \cdot e^{jk_m x}$$

- calculating f_t and f_{xx}

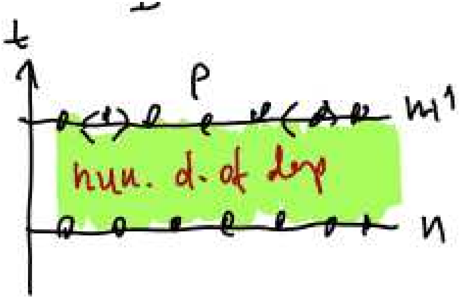
$$f(x,t) = e^{-\alpha \cdot k_m^2 t} \cdot \phi(x)$$

- initial condition decays with time
- each component (of $\phi(x)$) decays exponentially with time, but each component decays at a (different) rate depending on the square of its individual wave number (k_m)
- distribution changes in time

1. dicretizing - create a space grid
2. approximating exact derivatives in PDE by a finite difference approximation (FDA)
3. substitute FDA into PDE to obtain algebraic finite difference equation (FDE)
4. solve resulting algebraic FDEs

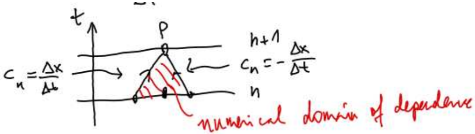
- implicit methods
- numerical information propagation speed

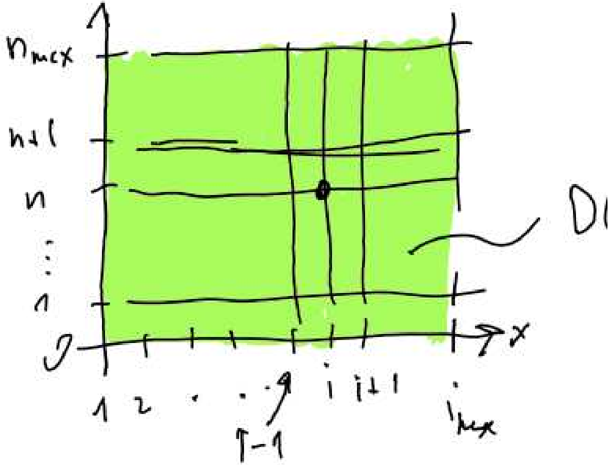
$$c_n = \frac{\Delta x}{\Delta t} \to \infty$$



- explicit methods
- numerical information propagation speed

$$c_n = \frac{\Delta x}{\Delta t} < \infty$$





- $D(x, y, z, t)$ is domain of solution (open domain in direction t)
- equidistant grid in both directions ($\Delta x \neq \Delta t$)
- some notations used later :

$$f(x_i, t^n) = f_i^n$$

$$\frac{\partial f(x_i, t^n)}{\partial t} = \left.\frac{\partial f}{\partial t}\right|_i^n = f_t|_i^n$$

$$\frac{\partial^2 f(x_i, t^n)}{\partial x^2} = \left.\frac{\partial^2 f}{\partial x^2}\right|_i^n = f_{xx}|_i^n$$

- use Taylor's series - first order forward time approximation

$$f_i^{n+1} = f_i^n + f_t|_i^n \cdot \Delta t + \frac{1}{2} f_{tt}|_i^n \cdot (\Delta t)^2 + \dots$$

$$f_t|_i^n = \frac{f_i^{n+1} - f_i^n}{\Delta t} + O(\Delta t)$$

- first order backward time approximation
- second order centered time approximation - using points at $n+1$ and $n+1/2$ using Taylor's series expansion

- at point $i+1$,n :

$$f^n_{i+1} = f^n_i + f_x|^n_i \cdot \Delta x + \frac{1}{2}\, f_{xx}|^n_i \cdot \Delta x^2 + \frac{1}{6}\, f_{xxx}|^n_i\, \Delta x^3 + \frac{1}{24}\, f_{xxxx}|^n_i\, \Delta x^4 + \ldots$$

$$f^n_{i-1} = f^n_i - f_x|^n_i \cdot \Delta x + \frac{1}{2}\, f_{xx}|^n_i \cdot \Delta x^2 - \frac{1}{6}\, f_{xxx}|^n_i\, \Delta x^3 + \frac{1}{24}\, f_{xxxx}|^n_i\, \Delta x^4 + \ldots$$

- adding up : $\boxed{f_x|^n_i = \frac{f^n_{i+1} - f^n_{i-1}}{2 \cdot \Delta x}}$

- substracting : $\boxed{f_{xx}|^i_i = \frac{f^n_{i+1} - 2f^n_i + f^n_{i-1}}{\Delta x}}$

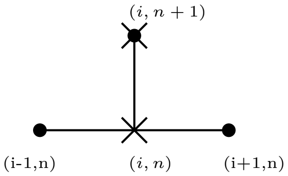
- solve $f_t = \alpha \cdot f_{xx}$ with $f(x,0) =$ known and $f(0,t)$ and $f(L,t)$ known
- use forward approximation for time and center approximation for space

$$\frac{f_i^{n+1} - f_i^n}{\Delta t} = \alpha \cdot \frac{f_{i+1}^n - 2f_i^n + f_{i-1}^n}{\Delta x^2}$$

- explicit scheme :

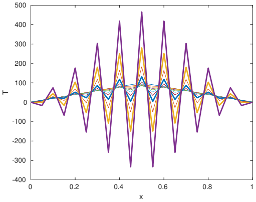
$$\boxed{f_i^{n+1} = f_i^n + d \cdot (f_{i+1}^n - 2f_i^n + f_{i-1}^n)}$$

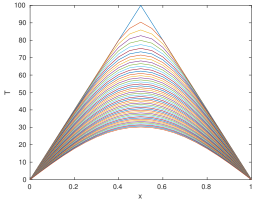
- where $d = \alpha \cdot \frac{\Delta t}{\Delta x^2}$ is diffusion number



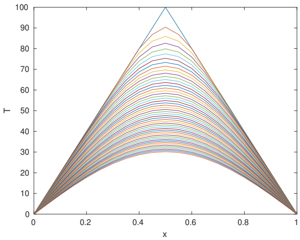
- diffusion number (d) - controls stability
- if d is too high - physically impossible solutions occur

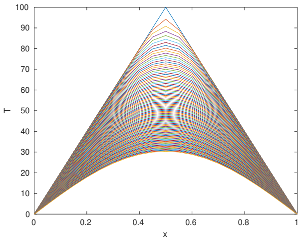
  numerically unstable
- boundary of stability : $d \leq 0.5$
- a finer grid means a more smaller time step to stay in stability region
- numerical information speed $c_n = \frac{\Delta x}{\Delta t}$, so numerically information propagates (in FTCS) one physical grid increment in all directions during each time step





- approximation is explicit
- single step solution
- consistent
- $O(\Delta t) + O(\Delta x^2)$
- conditionally stable : $d = \alpha \cdot \Delta t/(\Delta x)^2$ and $d \leq 0.5$
- convergent





- Richardson (Leapfrog) method
- for f_t use three-level second-order centered-difference approximation

$$f_i^{n+1} = f_i^n + f_t|_i^n \, \Delta t + \dots \qquad \text{and} \qquad f_i^{n-1} = f_i^n - f_t|_i^n \, \Delta t + \dots$$

-

$$f_t|_i^n = \frac{f_i^{n+1} - f_i^{n-1}}{2\Delta t} = \alpha \cdot \frac{f_{i+1}^n - 2f_i^n + f_{i-1}^n}{\Delta x^2}$$

$$\boxed{f_i^{n+1} = f_i^{n-1} + 2d \cdot \left(f_{i+1}^n - 2f_i^n + f_{i-1}^n\right)}$$

- unconditionally unstable
- Leapfrog-method is useful when used on hyperbolic PDEs

- modification to the Richardson-method
- use for f_i^n in $f_{xx}|_i^n$

$$f_i^n = \frac{1}{2}\left(f_i^{n+1} + f_i^{n-1}\right)$$

$$\frac{f_i^{n+1} - f_i^{n-1}}{2\Delta t} = \alpha \cdot \frac{f_{i+1}^n - \left(f_i^{n+1} + f_i^{n-1}\right) + f_{i-1}^n}{\Delta x^2}$$

$$(1+2d)f_i^{n+1} = (1-2d)\cdot f_i^{n-1} + 2d(f_{i+1}^n + f_{i-1}^n)$$

- unconditionally stable, but
- using approximations substituting back to PDE, and in case of $\Delta t \to 0$ and $\Delta x \to 0$ it becomes indeterminate. So scheme is inconsistent.

- in explicit methods
  - inconsistency and conditional stability occurs
  - conditional stability causes too small stepsize

$$d = \alpha \cdot \frac{\Delta t}{\Delta x^2} < 0.5$$

  - too much computing effort
- implicit methods involves $n+1$ values in approximation
- unconditionally stable
- step size is limited by accuracy
- system of finite difference equations must be solved at each time level (time step)
- BTCS and Crank-Nicholson scheme

- fully implicit

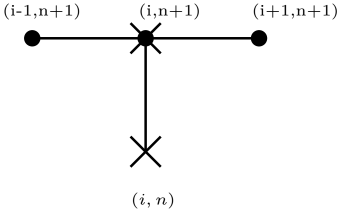
$$f_i^n = f_i^{n+1} + f_t\big|_i^{n+1} \cdot (-\Delta t) + \frac{1}{2} f_{tt}\big|_i^{n+1} (-\Delta t)^2 + \dots$$

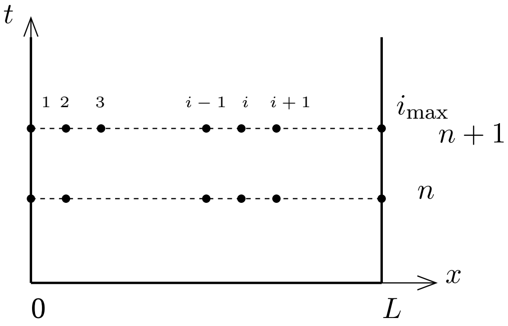
$$f_t\big|_i^{n+1} = \frac{f_i^{n+1} - f_i^n}{\Delta t} + O(\Delta t^2)$$

- $$\frac{f_i^{n+1} - f_i^n}{\Delta t} = \alpha \cdot \frac{f_{i+1}^{n+1} - 2f_i^{n+1} + f_{i-1}^{n+1}}{\Delta x^2}$$

$$-d \cdot f_{i-1}^{n+1} + (1 + 2d) f_i^{n+1} - d \cdot f_{i+1}^{n+1} = f_i^n$$

$$\text{using } d = \alpha \cdot \frac{\Delta t}{\Delta x^2}$$





- define grid in space:

$$x = \{x_1, x_2, \dots x_{i_{\max}}\} = \{x_i\}, i = 1, \dots i_{\max}$$

- time levels n and $n+1$
- for interior points :

$$-d \cdot f_{i-1}^{n+1} + (1+2d) f_i^{n+1} - d f_{i+1}^{n+1} = f_i^n$$

- boundary points ($i = 1$ and $i = i_{\max}$)

$$f_1^{n+1} = f_{BC}(0,t) \quad \text{and} \quad f_{i_{\max}}^{n+1} = f_{BC}(L,t)$$

$f_{BC}(x,t)$ describes temperature at both ends

- express f_i^{n+1} and f_i^n using $f_i^{n+1/2}$

$$f_i^{n+1} = f_i^{n+1/2} + f_t\big|_i^{n+1/2} \cdot \left(\frac{\Delta t}{2}\right) + O(\Delta t^2); \qquad f_i^{n} = f_i^{n+1/2} - f_t\big|_i^{n+1/2} \cdot \left(\frac{\Delta t}{2}\right) + O(\Delta t^2)$$

$$f_t\big|_i^{n+1/2} = \frac{f_i^{n+1} - f_i^n}{\Delta t}$$

- space derivatives expressed using n and $n+1$ levels

$$f_{xx}\big|_i^{n+1/2} = \frac{1}{2}\left(f_{xx}\big|_i^{n} + f_{xx}\big|_i^{n+1}\right)$$

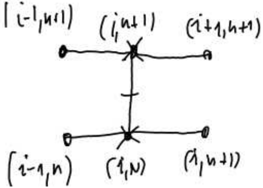
- collect terms

$$\frac{f_i^{n+1} - f_i^n}{\Delta t} = \alpha\left(\frac{f_{i+1}^{n+1} - 2f_i^{n+1} + f_{i-1}^{n+1}}{\Delta x^2} + \frac{f_{i+1}^{n} - 2f_i^{n} + f_{i-1}^{n}}{\Delta x^2}\right)$$

- expressed FDE (Finite Difference Equation) line for interior point

$$-d\cdot f_{i-1}^{n+1}+2(1+d)f_i^{n+1}-d\cdot f_{i-1}^{n+1} = d\cdot f_{i-1}^{n}+2(1-d)f_i^{n}+d\cdot f_{i+1}^{n}$$

$$\text{where } d = \alpha \cdot \frac{\Delta t}{\Delta x^2}$$



Derivative BCs

- Neumann-type boudnary conditions, like

$$\frac{\partial T}{\partial x}(L, t) = 0$$

- change in space derivative side
- in case of FTCS : $(i = I)$ is boundary

$$f_I^{n+1} = f_I^n + d \cdot \left(f_{I-1}^n - 2f_I^n + f_{I+1}^n\right)$$

- f_{I+1}^n is outside of domain

$$f_x|_I^n = \frac{f_{I+1}^n - f_{I-1}^n}{2 \cdot \Delta x}$$

$$\text{from above : } f_I^{n+1} = f_I^n + d \cdot \left\{f_{I-1}^n - 2f_I^n + \left(f_{I-1}^n + 2\Delta x \cdot f_x|_I^n\right)\right\}$$

$$\boxed{f_I^{n+1} = 2d \cdot f_{I-1}^n + (1-2d)f_I^n + 2d \cdot \Delta x \cdot f_x|_I^n}$$