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Computer Modelling Techniques

Numerical Methods
Lecture 4: Solution of 1D unsteady diffusion equation

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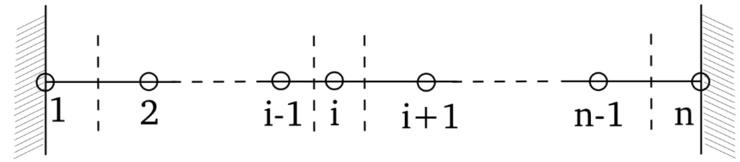
Recap

Steady-state diffusion equation, for example heat conduction:

$$1D: \quad \frac{d}{dx}\left(\lambda\frac{dT}{dx}\right) + S(x,T) = 0$$

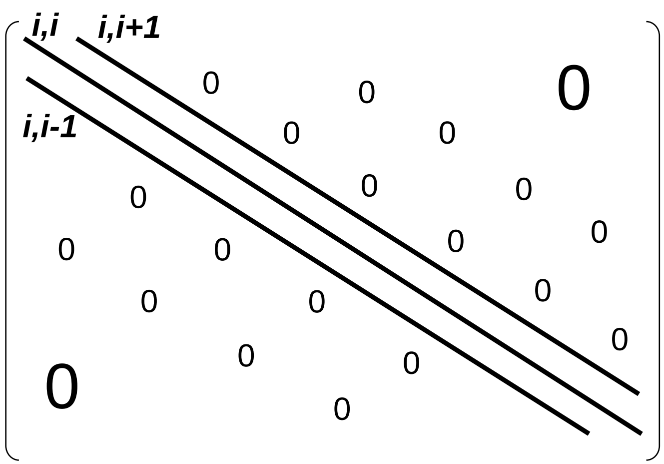


FV

$$a_W T_W + a_P T_P + a_E T_E = b$$

$$a_W = -\frac{\lambda_w}{\delta x_w}, \qquad a_P = \frac{\lambda_w}{\delta x_w} + \frac{\lambda_e}{\delta x_e} - S_P \Delta x, \qquad a_E = -\frac{\lambda_e}{\delta x_e}, \qquad b = S_C \Delta x$$

A=



A×**T**=**B**: linear algebraic system with n equations

A: *n*×*n* tridiagonal matrix; **T**,**B**: *n*×*1* vectors

T=A\B

Steady-state: we solve the system only once

And what about unsteady equations?

Today’s menu

- Finite-volume method for unsteady PDE
- Explicit time-scheme
- Crank-Nicolson time-scheme
- Fully-implicit time-scheme
- Seminar 3 – solution of 1D unsteady heat equation with Matlab (demo 3)

Expected outcome: know the principles of time-marching algorithms for the solution of unsteady PDEs; know and be able to implement implicit/explicit time-schemes; use matlab to obtain the numerical solution.

The temporal discretisation concept

The unsteady diffusion equation involves a first-order time-derivative, e.g. 1D unsteady heat conduction:

$$\frac{\partial\left(\rho c_p T\right)}{\partial t} = \frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x}\right) + S(x,t,T)$$

When the time-derivative is first-order, the equation has a **parabolic behavior** with time: disturbances travel only towards the $+t$ direction, and not backward ($-t$).

Only one temporal boundary condition is required: the **initial condition** $T(x, t = 0)$.

The solution in time is obtained by **time-marching**: the solution at any time $t + \Delta t$ is found by advancing the solution from time t, no need to know what happens at times $t > t + \Delta t$.

Solution procedure:

$t = 0$: we need a known **initial condition**, $T(x, t = 0)$

$t = 1\Delta t$: discretisation of the equation → linear system → solution → $T(x, t = 1\Delta t)$

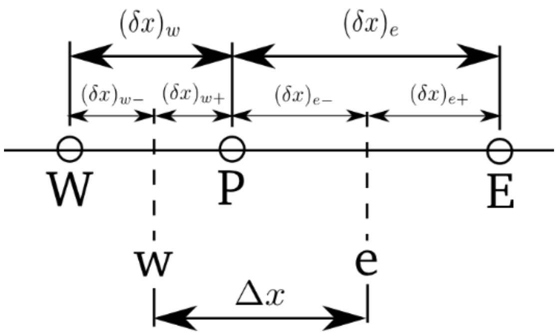
$t = 2\Delta t$: $T(x, t = 1\Delta t)$ is our new initial condition → linear system → solution → $T(x, t = 2\Delta t)$

$t = t_{final}$: $T(x, t = t_{final})$

→ At every time step, we need to solve a new linear system

The unsteady finite-volume method – 1D

Equation to be solved:
1D unsteady heat conduction (here with $S(x,t)=0$)



$$\frac{\partial(\rho c_p T)}{\partial t} = \frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x}\right)$$

Integration in space and time (ρ,c_p constant):

$$\rho c_p \int_t^{t+\Delta t} \int_V \frac{\partial T}{\partial t} dV dt = \int_t^{t+\Delta t} \int_V \frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x}\right) dV dt$$

Discretisation of the single terms:

$$\rho c_p \int_t^{t+\Delta t} \int_V \frac{\partial T}{\partial t} dV dt = \rho c_p \int_w^e \left[\int_t^{t+\Delta t} \frac{\partial T}{\partial t} dt\right] A dx = \rho c_p (T_P^1 - T_P^0) A \Delta x$$

T_P^0: T_P at time t, T_P^1: T_P at time $t+\Delta t$

$$\int_t^{t+\Delta t} \int_V \frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x}\right) dV dt = \int_t^{t+\Delta t} \int_w^e \frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x}\right) A dx\, dt = \int_t^{t+\Delta t} \left[\lambda_e \frac{T_E - T_P}{\delta x_e} - \lambda_w \frac{T_P - T_W}{\delta x_w}\right] A dt$$

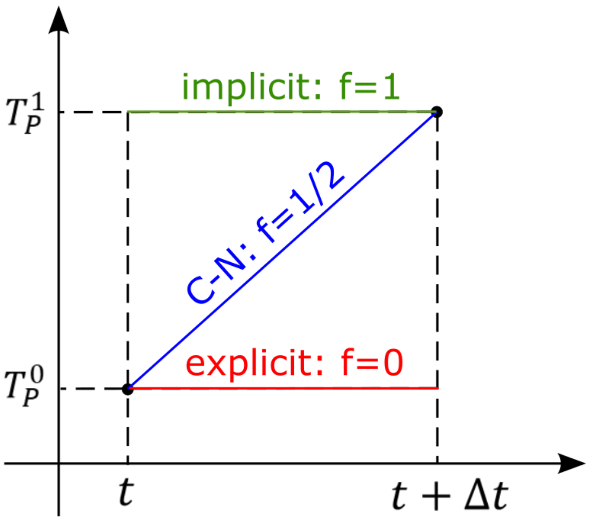
Now, integration in time requires a **profile assumption** for *T(t)* between *t* and *t+Δt*

The unsteady finite-volume method – 1D

Now, integration in time requires a **profile assumption** for *T(t)* between *t* and *t+Δt.*

The integral will be a function of T_P^0 and T_P^1. Easiest solution: a linear profile!

$$\int_t^{t+\Delta t} T_P dt = [fT_P^1 + (1-f)T_P^0]\Delta t$$

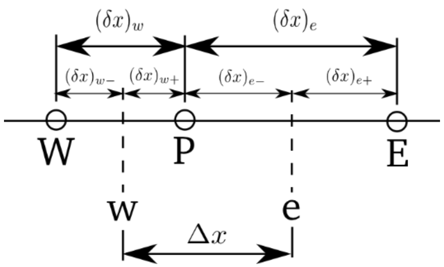


- ***f=0*** → **explicit scheme**: 1st order accurate, conditionally stable
- ***f=1*** → **fully-implicit scheme**: 1st order accurate, unconditionally stable
- ***f=1/2*** → **Crank-Nicolson scheme**: 2nd order accurate, conditionally stable

$$\rho c_p (T_P^1 - T_P^0)\Delta x = \left\{ f\left[\lambda_e \frac{T_E^1 - T_P^1}{\delta x_e} - \lambda_w \frac{T_P^1 - T_W^1}{\delta x_w}\right] + (1-f)\left[\lambda_e \frac{T_E^0 - T_P^0}{\delta x_e} - \lambda_w \frac{T_P^0 - T_W^0}{\delta x_w}\right]\right\}\Delta t$$

The unsteady finite-volume method – 1D

(superscript *1* is here dropped)



$$-f\frac{\lambda_w}{\delta x_w}T_W+\left[\rho c_p\frac{\Delta x}{\Delta t}+f\left(\frac{\lambda_w}{\delta x_w}+\frac{\lambda_e}{\delta x_e}\right)\right]T_P-f\frac{\lambda_e}{\delta x_e}T_E=$$

$$=\rho c_p\frac{\Delta x}{\Delta t}T_P^0+(1-f)\left[\frac{\lambda_w}{\delta x_w}T_W^0+\frac{\lambda_e}{\delta x_e}T_E^0-\left(\frac{\lambda_w}{\delta x_w}+\frac{\lambda_e}{\delta x_e}\right)T_P^0\right]$$

Final linear equation

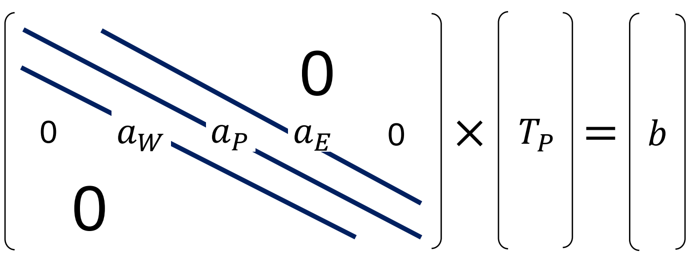
$$a_W T_W + a_P T_P + a_E T_E = b$$

$$a_W=-f\frac{\lambda_w}{\delta x_w}\qquad a_E=-f\frac{\lambda_e}{\delta x_e}$$

$$a_P=\rho c_p\frac{\Delta x}{\Delta t}+f\left(\frac{\lambda_w}{\delta x_w}+\frac{\lambda_e}{\delta x_e}\right)$$

$$b=\rho c_p\frac{\Delta x}{\Delta t}T_P^0+(1-f)\left[\frac{\lambda_w}{\delta x_w}T_W^0+\frac{\lambda_e}{\delta x_e}T_E^0-\left(\frac{\lambda_w}{\delta x_w}+\frac{\lambda_e}{\delta x_e}\right)T_P^0\right]$$

Assembling the system and advancing the solution in time



A×T=B: linear algebraic system with ***n*** equations
A: **tridiagonal** *n*×*n* matrix, **T**,**B**: *n*×*1* vectors

The system is solved for $t=\Delta t$, $2\Delta t$, $3\Delta t$, …, till t_{end}

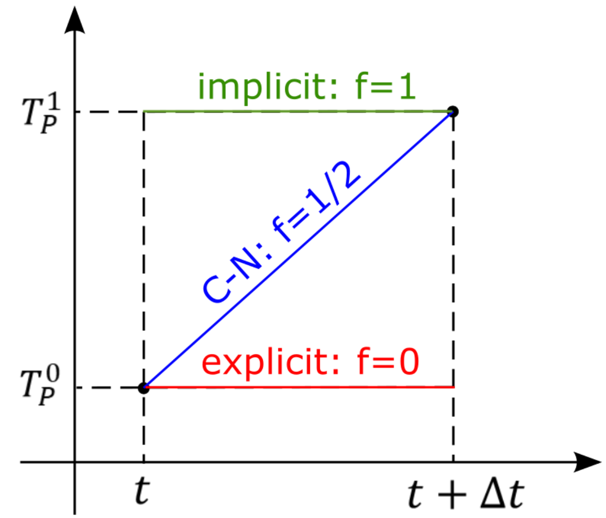
When $t=\Delta t$: T^0 in vector ***B*** is the **initial condition**

When $t>\Delta t$: T^0 in vector ***B*** is the **solution at the previous time instant**

Explicit time-scheme

Can be derived from the previous equations by setting $f = 0$:

$$\int_t^{t+\Delta t} T_P dt = T_P^0 \Delta t$$



Coefficients: $a_P = \rho c_p \dfrac{\Delta x}{\Delta t}, \qquad a_E = 0, \qquad a_W = 0$

$$b = \frac{\lambda_w}{\delta x_w} T_W^0 + \frac{\lambda_e}{\delta x_e} T_E^0 - \left(\frac{\lambda_w}{\delta x_w} + \frac{\lambda_e}{\delta x_e} - \rho c_p \frac{\Delta x}{\Delta t} \right) T_P^0$$

Stability condition: coefficient for T_P^0 when at LHS must be negative (remember L1, slide 15)

$$\longrightarrow \left(\frac{\lambda_w}{\delta x_w} + \frac{\lambda_e}{\delta x_e} - \rho c_p \frac{\Delta x}{\Delta t} \right) < 0$$

Example: $\lambda_w = \lambda_e, \delta x_w = \delta x_e = \Delta x$ $\longrightarrow$ $\Delta t < \dfrac{\rho c_p (\Delta x)^2}{2\lambda}$

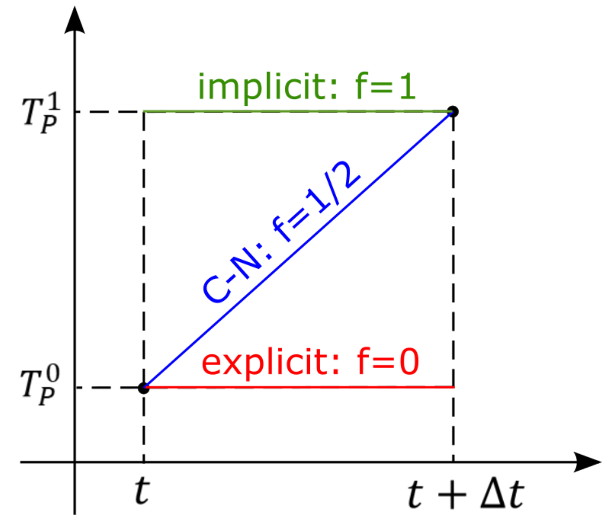
- $\Delta t_{max} \propto (\Delta x)^2$: if we refine the grid we must **exponentially** decrease the time step!
- Equations for each CV are decoupled $\longrightarrow$ no need to solve a system of equations
- It's a 1st-order scheme, so accuracy is still limited

Note: LHS means left-hand side of discretization equation

Crank-Nicolson time-scheme

Can be derived from the previous equations by setting $f = 1/2$:

$$\int_{t}^{t+\Delta t} T_P dt = \frac{T_P^1 + T_P^0}{2} \Delta t$$



$$a_P = \rho c_p \frac{\Delta x}{\Delta t} + \frac{1}{2}\left(\frac{\lambda_w}{\delta x_w} + \frac{\lambda_e}{\delta x_e}\right)$$

$$a_E = -\frac{1}{2}\frac{\lambda_e}{\delta x_e}, \qquad a_W = -\frac{1}{2}\frac{\lambda_w}{\delta x_w}$$

$$b = \frac{1}{2}\left[\frac{\lambda_w}{\delta x_w} T_W^0 + \frac{\lambda_e}{\delta x_e} T_E^0 - \left(\frac{\lambda_w}{\delta x_w} + \frac{\lambda_e}{\delta x_e} - 2\rho c_p \frac{\Delta x}{\Delta t}\right) T_P^0\right]$$

Stability condition: $\Delta t < \frac{\rho c_p (\Delta x)^2}{\lambda}$

- Stability condition still severe; larger Δt are still possible, but may give rise to oscillations
- 2nd-order accurate in time: if the time step is small (stable), it is the most accurate scheme
- Requires solution of a linear system, thus more complicated then time-explicit

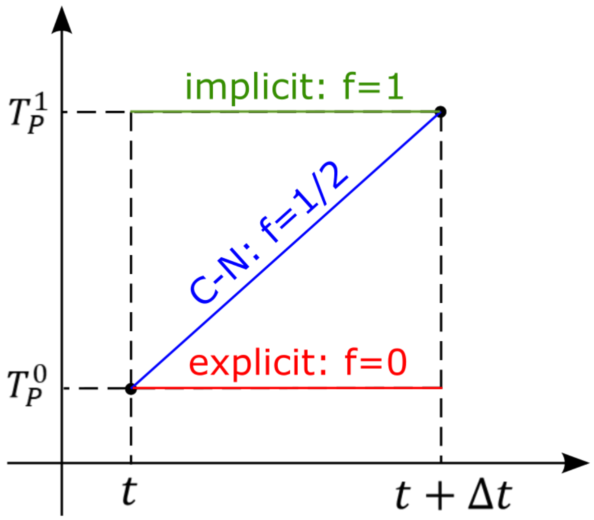
Fully-implicit time-scheme

Can be derived from the previous equations by setting $f = 1$:

$$\int_t^{t+\Delta t} T_P dt = T_P^1 \Delta t$$

$$a_P = \rho c_p \frac{\Delta x}{\Delta t} + \frac{\lambda_w}{\delta x_w} + \frac{\lambda_e}{\delta x_e}$$

$$a_E = -\frac{\lambda_e}{\delta x_e}, \qquad a_W = -\frac{\lambda_w}{\delta x_w}, \qquad b = \rho c_p \frac{\Delta x}{\Delta t} T_P^0$$



Stability condition: $-\rho c_p \frac{\Delta x}{\Delta t} < 0$ → **Always respected!**

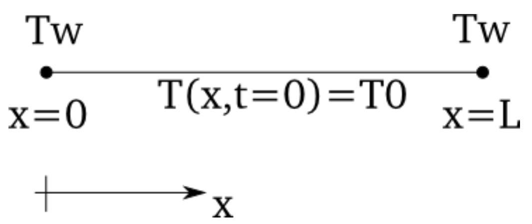
- The fully-implicit time scheme is stable for any size of time step
- It's a 1st-order scheme, so accuracy is still limited
- Requires solution of a linear system, thus more complicated then time-explicit

What to take home from today's lecture

- How to discretise the 1D unsteady heat conduction equation using FV
- Advantages/limits of explicit, fully-implicit and Crank-Nicolson schemes
- How to derive the condition for the numerical stability of the time-marching algorithm
- How to use Matlab to solve unsteady problems

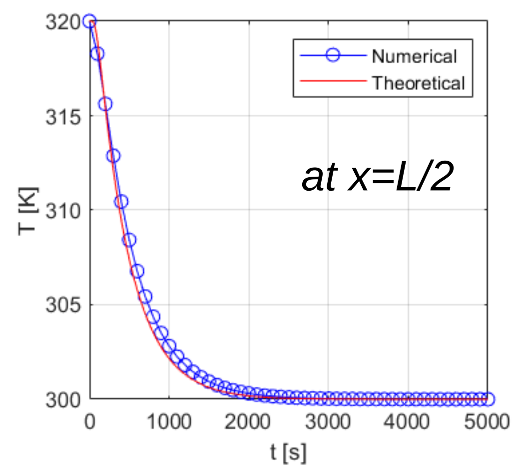
Worked example 1

Implement a FV code in Matlab to solve a 1D unsteady heat conduction problem, using the fully-implicit method.



Parameters:

- L=1 m
- n=21 equidistant nodes
- λ=400 W/(m·K), ρ=4000 kg/m^3, c_p=400 J/(kg · K)
- T(x=0)=T(x=L)=T_w=300 K
- Initial condition T(x,t=0)=T_0=320 K
- Time-step size Δt=100 s
- End time of simulation t_{end}=5000 s



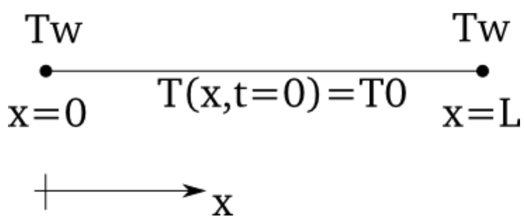
Compare your results with the following analytical solution:

$$T(x,t) = T_w + \frac{2(T_0 - T_w)}{\pi}\sum_{i=1}^{\infty}\frac{\left[1-(-1)^i\right]}{i}e^{-\alpha\mu_i^2 t}\sin(\mu_i x) \qquad \mu_i = \frac{i\pi}{L}, \alpha = \frac{\lambda}{\rho c_p}$$

Worked example 1

There will be $t_{end}/\Delta t$=5000/100=50 time-steps.

At every k-th time-step:



1st CV: $a_{1,P}T_{1,P} + a_{1,E}T_{1,E} = b_1 \;\Rightarrow\; a_{1,1}T_1 + a_{1,2}T_2 = b_1$

$\Rightarrow \quad a_{1,1} = 1, \qquad a_{1,2} = 0, \qquad b_1 = T_w$

ith CV: $a_{i,W}T_{i,W} + a_{i,P}T_{i,P} + a_{i,E}T_{i,E} = b_i \;\Rightarrow\; a_{i,i-1}T_{i-1} + a_{i,i}T_i + a_{i,i+1}T_{i+1} = b_i$

$$\Rightarrow \quad a_{i,i-1} = -f\frac{\lambda}{\delta x}, \qquad a_{i,i} = \rho c_p\frac{\Delta x}{\Delta t} + f\frac{2\lambda}{\delta x}, \qquad a_{i,i+1} = -f\frac{\lambda}{\delta x}$$

$$b_i = \rho c_p\frac{\Delta x}{\Delta t}T_i^{k-1} + (1-f)\left[\frac{\lambda}{\delta x}T_{i-1}^{k-1} + \frac{\lambda}{\delta x}T_{i+1}^{k-1} - \frac{2\lambda}{\delta x}T_i^{k-1}\right]$$

nth CV: $a_{n,W}T_{n,W} + a_{n,P}T_{n,P} = b_n \;\Rightarrow\; a_{n,n-1}T_{n-1} + a_{n,n}T_n = b_n$

$\Rightarrow \quad a_{n,n-1} = 0, \qquad a_{n,n} = 1, \qquad b_n = T_w$

The system is solved for *t=Δt, 2Δt, …, kΔt, …,* till t_{end}

When ***t=Δt***: $\boldsymbol{T^{k-1}}$ in b_i is the **initial condition**

When ***t>Δt***: $\boldsymbol{T^{k-1}}$ in b_i is the **solution at the previous time instant**