

Solvers, Approximation, Stability, Boundedness of Numerical schemes

Remark: foils with „black background“ could be skipped, they are aimed to the more advanced courses

SOLVERS

FEM, BEM, FVM, FD transfer PDE into system of algebraic equations for T_j (nodal pressures, velocities, temperature, concentrations...) solved by

➤ Finite methods (Gauss, [SVD](#), [LU decomposition](#), [frontal](#) methods)
 N^3 operations are required – suitable for smaller systems.

➤ Iterative methods ([GS](#), [multigrid](#), [GMRES](#), conjugated gradients).
Prevails at CFD calculations, characterized by number cells (nodes) of several millions and parallel processing (external as well as internal aerodynamics of cars requires up to 10^8 finite volumes, solved in clusters of e.g. 512 and more processors)

Iterative methods are not so sensitive to round-off errors (that's why they can be applied for such huge systems)

Mathematical Requirements

Three Mathematical requirements

➤ **consistency** (discretized equation for $\Delta t \rightarrow 0, \Delta h \rightarrow 0$ must be identical with PDE)

$$T_{numerical} = T + O(\Delta t^m, \Delta h^n) \quad \text{order of accuracy (m-with respect time, n-with respect to spatial approximation)}$$
$$O(\Delta t^m, \Delta h^n) < K\Delta t^m + L\Delta h^n$$

➤ **stability** (attenuation of round-off errors or glitches of initial conditions)

➤ **convergency**. Lax theorem: consistent and stable numerical scheme converges to exact solution (but it holds only for linear systems)

Physical Requirements

Three Physical requirements

➤ **Conservativeness**. Balance of mass should hold exactly at an element level and globally. Fulfilled by FVM (Finite Volume Method). Not exactly satisfied by FEM.

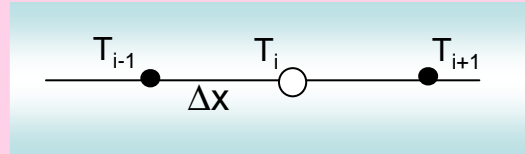
➤ **Boundedness**. Solution should not exhibit local min/max in the absence of internal sources (of mass, momentum or heat). Solution should be bounded by boundary values. Min/max principle.

➤ **Transportiveness**. Numerical scheme should reflect directionality of information transfer (convection along streamlines)

Numerical method-analysis

Few examples, how to analyze order of accuracy and stability of suggested numerical schemes (FD methods)

Order of accuracy



Taylor expansion

$$T_{i+1} = T_i + \frac{dT_i}{dx} \Delta x + \frac{1}{2} \frac{d^2 T_i}{dx^2} \Delta x^2 + \frac{1}{6} \frac{d^3 T_i}{dx^3} \Delta x^3 + O(\Delta x^4)$$

$$T_{i-1} = T_i - \frac{dT_i}{dx} \Delta x + \frac{1}{2} \frac{d^2 T_i}{dx^2} \Delta x^2 - \frac{1}{6} \frac{d^3 T_i}{dx^3} \Delta x^3 + O(\Delta x^4)$$

Approximation of first derivative

$$\frac{dT}{dx}(x_i) \cong \frac{T_{i+1} - T_{i-1}}{2\Delta x} = \frac{dT}{dx}(x_i) + \frac{d^3 T}{dx^3}(x_i) \frac{\Delta x^2}{3} + \text{HOT}$$

Higher Order Terms

Accurate for 2nd order polynomials $T=1, x, x^2$

$$\frac{dT}{dx}(x_i) \cong \frac{T_i - T_{i-1}}{\Delta x} = \frac{dT}{dx}(x_i) - \frac{d^2 T}{dx^2}(x_i) \frac{\Delta x}{2} + \text{HOT}$$

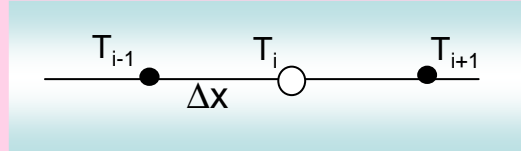
Accurate for 1st order polynomials $T=1, x$

Approximation of second derivative

$$\frac{d^2 T}{dx^2}(x_i) \cong \frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta x^2} = \frac{d^2 T}{dx^2}(x_i) + \frac{d^4 T}{dx^4}(x_i) \frac{\Delta x^2}{12} + \text{HOT}$$

Accurate for 3rd order polynomials $T=1, x, x^2, x^3$

Order of accuracy



Therefore finite differences substituting derivatives at node x_i are

➤ First order $\frac{dT}{dx}(x_i) \cong \frac{T_i - T_{i-1}}{\Delta x}$

➤ Second order $\frac{dT}{dx}(x_i) \cong \frac{T_{i+1} - T_{i-1}}{2\Delta x}$

➤ Third order $\frac{d^2T}{dx^2}(x_i) \cong \frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta x^2}$

Stability example (explicit method)

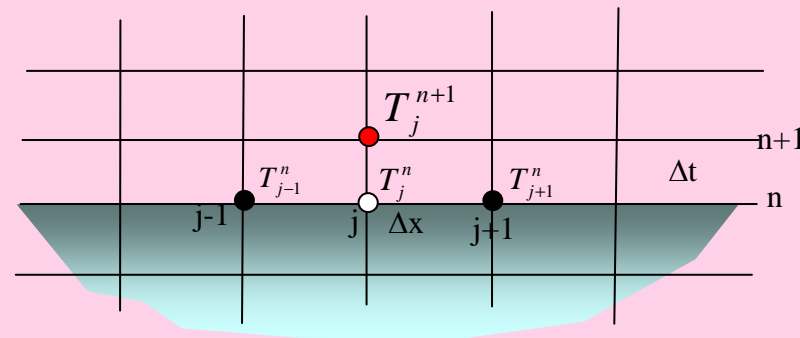
Unsteady heat transfer (Fourier equation – parabolic)

$$\frac{\partial T}{\partial t} = a \frac{\partial^2 T}{\partial x^2}$$

T-temperature, a -temperature diffusivity

Finite difference method **EXPLICIT** (explicit means that unknown temperatures at a new time level can be expressed explicitly, without necessity to solve a system of algebraic equations).

$$\frac{T_j^{n+1} - T_j^n}{\Delta t} = a \frac{T_{j-1}^n - 2T_j^n + T_{j+1}^n}{\Delta x^2}$$



What is the order of accuracy?

Stability example (explicit method)

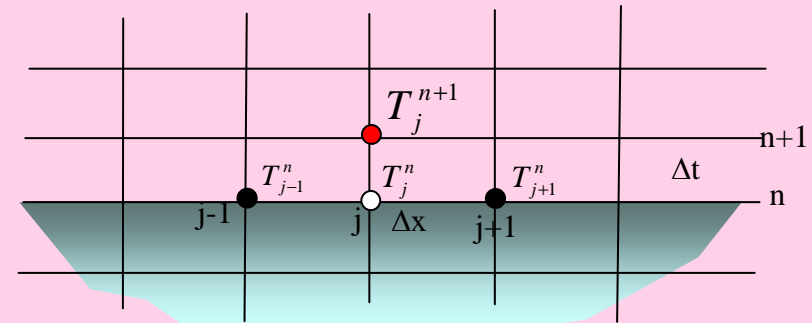
$$\frac{T_j^{n+1} - T_j^n}{\Delta t} = a \frac{T_{j-1}^n - 2T_j^n + T_{j+1}^n}{\Delta x^2}$$

$$\frac{\partial T}{\partial t} + O(\Delta t) = a \frac{\partial^2 T}{\partial x^2} + O(a\Delta x^3)$$

Residual of this PDE is therefore

$$res = O(\Delta t) + O(a\Delta x^3)$$

Scheme is consistent, linear with respect time, cubic with respect space.



Stability example (explicit method)

Rewrite the explicit formula to the following (explicit) form

$$T_j^{n+1} = \frac{a\Delta t}{\Delta x^2} T_{j-1}^n + \frac{a\Delta t}{\Delta x^2} T_{j+1}^n + \left(1 - \frac{2a\Delta t}{\Delta x^2}\right) T_j^n = AT_{j-1}^n + AT_{j+1}^n + (1 - 2A)T_j^n$$

Unknown temperature at a new time level

Known temperatures at "old" time level

$$A = \frac{a\Delta t}{\Delta x^2}$$

Rules:

- Sum of coefficients must be the same on the left and on the right side ($1=A+A+1-2A$). Why? A constant solution must be fulfilled exactly!
- All coefficients must be positive for bounded solution. Why?

Stability example (explicit method)

So why all coefficients must be positive for bounded solution?

Resulting value T is calculated as a weighted average of values (sum of weighting coefficients must be 1). Let us assume only two values for simplicity $T = AT_1 + (1 - A)T_2$

and $T_1 < T_2$. The solution is bounded if $T_1 < T < T_2$. Let us assume, that the result is **not** bounded and $T < T_1$. Then

$$AT_1 + (1 - A)T_2 < T_1$$

$$(1 - A)T_2 < T_1(1 - A)$$

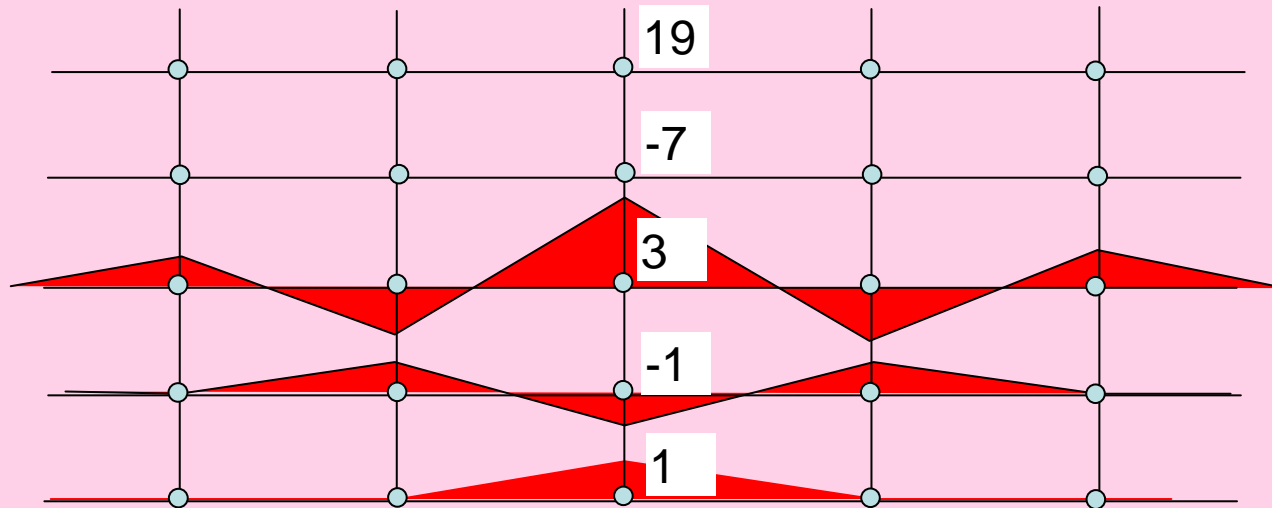
For positive value $(1 - A) > 0$ it follows that $T_1 > T_2$ and this is contradiction.

Stability example of unbounded solution

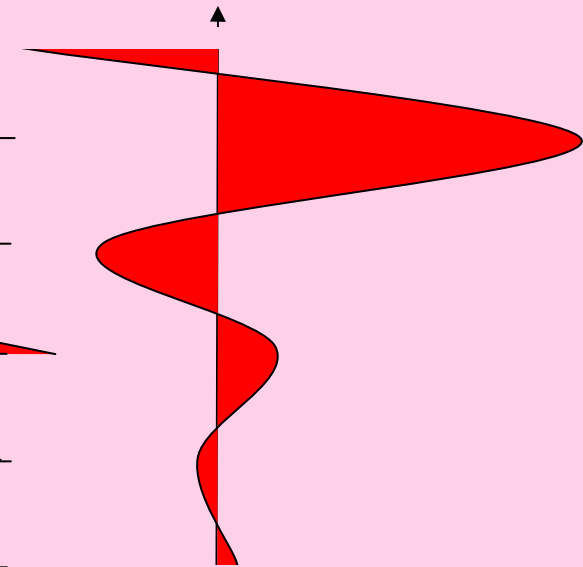
Let us consider what would happen if $A=1$ (negative value $1-2A$)

$$T_j^{n+1} = AT_{j-1}^n + AT_{j+1}^n + (1-2A)T_j^n$$

$$T_j^{n+1} = T_{j-1}^n + T_{j+1}^n - T_j^n$$



Initial condition is 0 in all nodes and only in one node is 1.



Evolution of initial condition in node

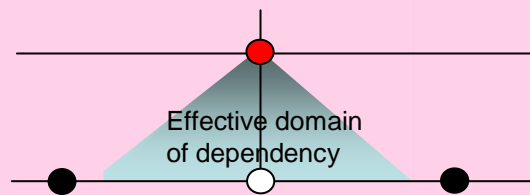
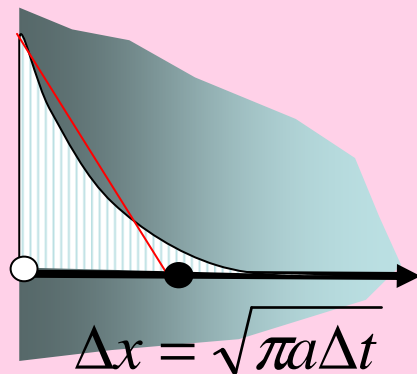
Stability example (explicit method)

Stability condition can be expressed as a restriction of time step

$$1 - 2A > 0 \quad A = \frac{a\Delta t}{\Delta x^2}$$

$$\Delta t < \frac{\Delta x^2}{2a}$$

Interpretation in terms of penetration theory. Effective velocity of a thermal pulse



Δx -distance of penetrated thermal pulse at a time Δt

$$\Delta t < \frac{\Delta x^2}{\pi a}$$

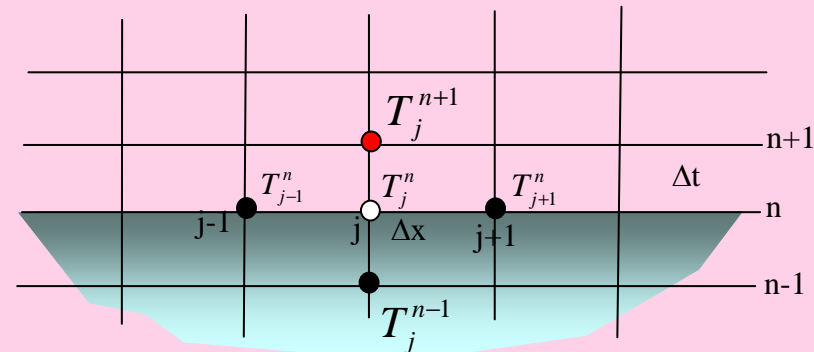
Stability example of wrong scheme

Richardson's scheme for the solution of previous equation

$$\frac{T_j^{n+1} - T_j^{n-1}}{2\Delta t} = a \frac{T_{j-1}^n - 2T_j^n + T_{j+1}^n}{\Delta x^2}$$

operates at 3 time levels, n-1, n, n+1
and has higher orders of accuracy

$$res = O(\Delta t^2) + O(a\Delta x^3)$$

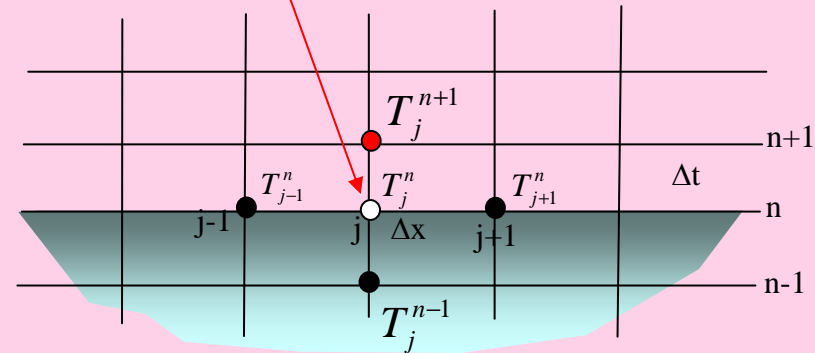


However, the scheme is practically useless. **WHY?**

Stability example of wrong scheme

Because this coefficient is always negative

$$T_j^{n+1} = T_j^{n-1} + 2A(T_{j-1}^n - 2T_j^n + T_{j+1}^n)$$



Stability how to improve Richardson?

Richardson's scheme

$$\frac{T_j^{n+1} - T_j^{n-1}}{2\Delta t} = a \frac{T_{j-1}^n - 2T_j^n + T_{j+1}^n}{\Delta x^2}$$

duFort Frankel scheme

$$\frac{T_j^{n+1} - T_j^{n-1}}{2\Delta t} = a \frac{T_{j-1}^n - T_j^{n+1} - T_j^{n-1} + T_{j+1}^n}{\Delta x^2}$$

$$T_j^{n+1} (1 + 2A) = T_j^{n-1} (1 - 2A) + 2A(T_{j-1}^n + T_{j+1}^n)$$

and this solution will be bounded for $A < 1/2$. Order of accuracy remains high.

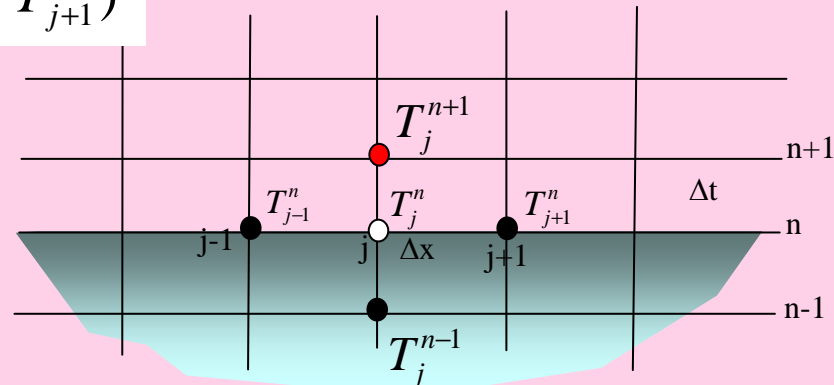
However:

Consistency with Fourier equation is assured only if $\lim_{\Delta x \rightarrow 0} \Delta t / \Delta x = 0$

otherwise the hyperbolic equation of heat transfer would be solved

$$\frac{\partial T}{\partial t} = a \frac{\partial^2 T}{\partial x^2} - \frac{a}{c^2} \frac{\partial^2 T}{\partial t^2}$$

where $c = \frac{\Delta x}{\Delta t}$



Stability Neumann

More precise (and more complicated) is the stability analysis suggested by von Neumann. It is based upon spectral decomposition of solution, i.e. at a time level n the spatial profile is substituted by Fourier expansion

$$T^n(x) = G_k^n e^{ik\pi x / \Delta x}$$

This Fourier component is substituted into differential equation and amplification factor G is evaluated. Numerical scheme is stable, as soon as the magnitude of identified amplification factor decreases.