Solvers, Approximation, Stability, Boundedness of Numerical schemes

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

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

  $$T_{\text{numerical}} = T + O(\Delta t^m, \Delta h^n)$$

  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.

- **Transportivness.** 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

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

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

Approximation of first derivative

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

\[ \text{Accurate for 2\textsuperscript{nd} order polynomials } T=1, x, x^2 \]

\[ \frac{dT}{dx} (x_i) \approx \frac{T_{i} - T_{i-1}}{\Delta x} = \frac{dT}{dx} (x_i) - \frac{d^2T}{dx^2} (x_i) \frac{\Delta x}{2} + \text{HOT} \]

\[ \text{Accurate for 1\textsuperscript{st} order polynomials } T=1, x \]

Approximation of second derivative

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

\[ \text{Accurate for 3\textsuperscript{rd} order polynomials } T=1, x, x^2, x^3 \]
Therefore finite differences substituting derivatives at node $x_i$ are

- **First order**
  \[
  \frac{dT}{dx}(x_i) \approx \frac{T_i - T_{i-1}}{\Delta x}
  \]

- **Second order**
  \[
  \frac{dT}{dx}(x_i) \approx \frac{T_{i+1} - T_{i-1}}{2\Delta x}
  \]

- **Third order**
  \[
  \frac{d^2T}{dx^2}(x_i) \approx \frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta x^2}
  \]
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).

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

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.
Rewrite the explicit formula to the following (explicit) form

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

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?
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.
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

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

\[ \Delta t < \frac{\Delta x^2}{2a} \]

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

\[ \Delta x = \sqrt{\pi a \Delta t} \]

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

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

\[
T_{j}^{n+1} (1 + 2A) = T_{j}^{n-1} (1 - 2A) + 2A(T_{j-1}^{n} + T_{j+1}^{n})
\]

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

However:

Consistency with Fourier equation is assured only if \( \lim_{\Delta t / \Delta x \to 0} \Delta t = 0 \)

otherwise the hyperbolic equation of heat transfer would be solved

\[
\frac{\partial T}{\partial t} = a \frac{\partial^2 T}{\partial x^2} - \frac{a \Delta x}{c^2} \frac{\partial^2 T}{\partial t^2}
\]

where \( c = \frac{\Delta x}{\Delta t} \)
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

$$T^n(x) = G^n_k e^{i k \pi x / \Delta x}$$

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.