Numerical Approximation

Solution of PDE

Analytical	•exact solution •only known for simple geometry •for practical projects not relevant •e.g. for verificaton of numerical models or research reasons
Physical	•very expensive •physical models were important before computer era •still important for parameter identification and verification
numerical	•state of art since more or less 15 years •very flexible and cheap •a lot of methods available, but FEM or FD are the most common methods

But: no model can be better than its input data

Numerical Methods

Analytical solution of a PDE with boundary (and initial) conditions is a function, which descripes the unknown variable in the total model area exactly.

„Computer can not find any function“.

Computer can solve discrete equations (Ax=b).

Discrete methods transfer PDE in discrete equations,
which can be solved by solvers.

Diskrete Methods

1. principle: The mathematical problem is solved in collocation points exactly, between them interpolation of solution.

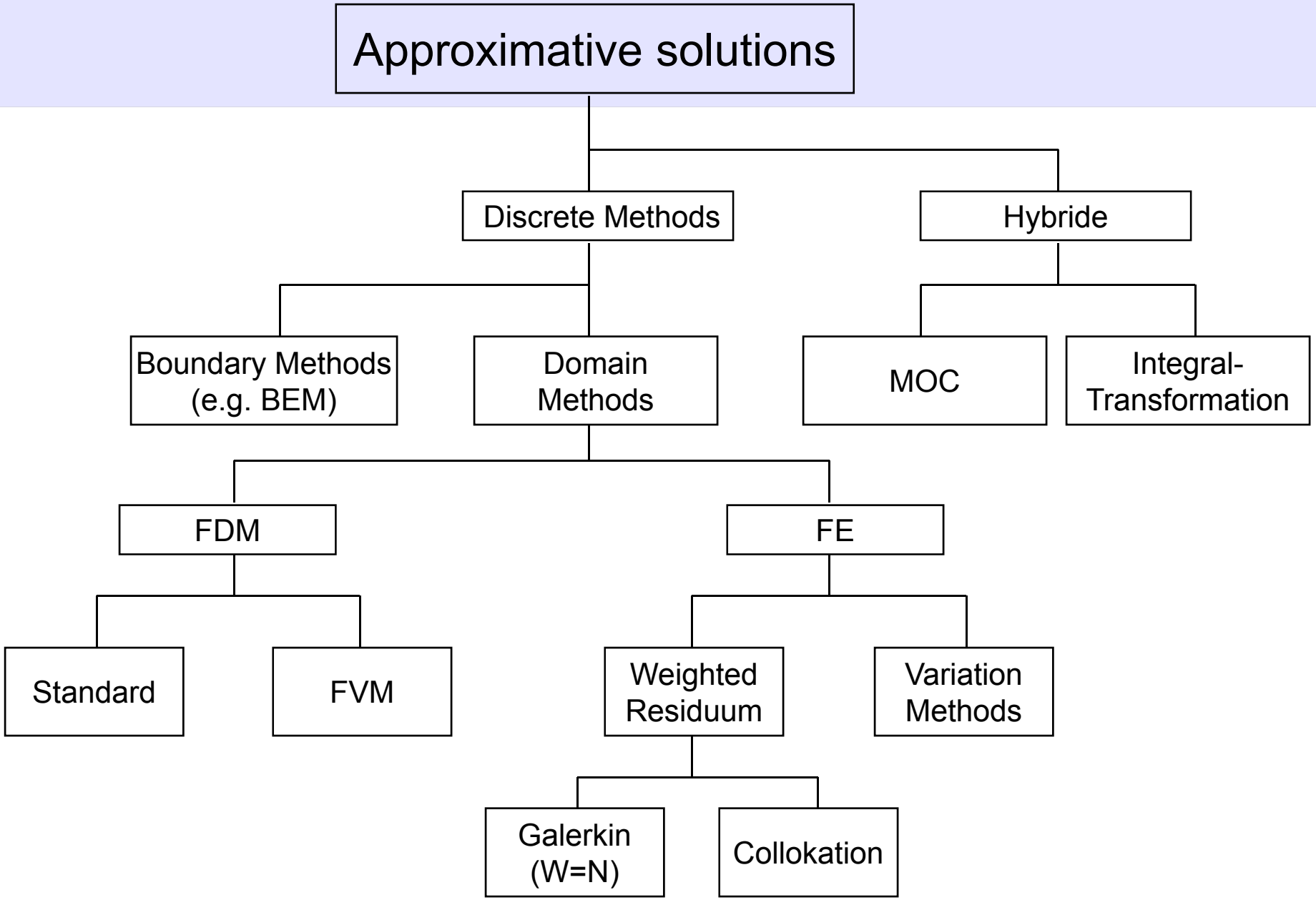
   Finite Elements
   Finite Differences
   Boundary Elements
   Finite Volume

   ⊢ biggest market share

2. principle: meshless methods don‘t need collocation points. Particles are followed, interaction is solved approximatly.

   Particel tracking Methods (Random walk, methods of characteristics)
   Lattice Gas Method

Futher: combinations, also with analytical methods

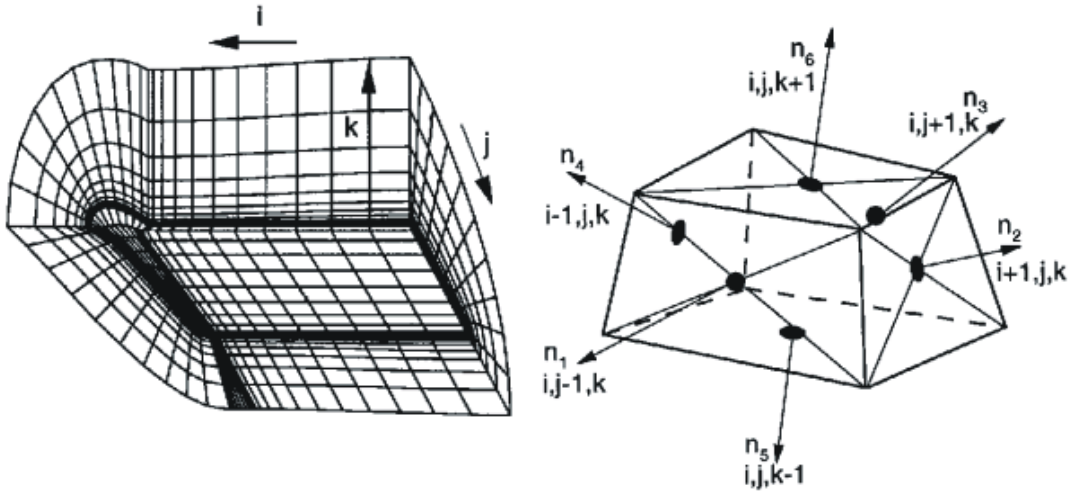


aus: Olaf Kolditz. Strömungsmechanik V/VI

Finite Volume

Modelarea is divided into cells (controll volumes) (mostly 4-edges in 2D, 6-sides in 3D), between them mass flux is balanced.

Values are defined in the centre of cells or at the edges, in-between interpolation.



Advantage

Mass balance is fulfilled localy and globaly,
more flexible discretization than FD

Disadvantage

Less flexible discretization than FEM
lower distribution than FDM und FEM, therefore less developed.

Method of Characteristics

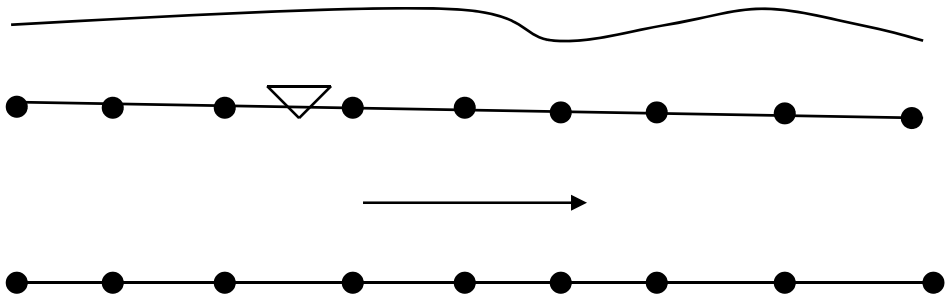
Particle-tracking-method, that means transport of a substance is described by a lot of particles moving in flow field.

Each transport step is devided in an advective and dispersive step.
Advection is simulated as movement of a tracer along a pathline.
Dispersion is calculated at the mesh and converted to the concentration of particles.

Advantage: stable soluation: no numerical dispersion, no oscillations

Disadvantage: Solution is not smooth, expensive

Boundary elements

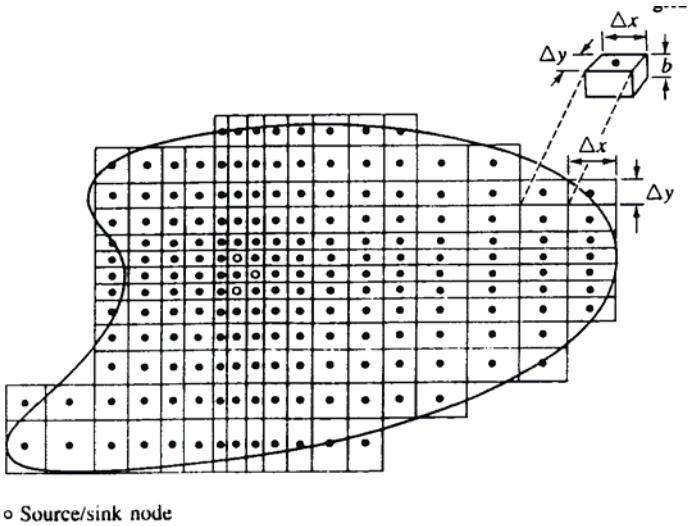


PDE is transverted into a boundary integral equation. On the base of the known analytical solution for point source in infinite space
(fundamental solution) the solution for the problem is interpolated for the individual boundary conditions.
Only boundaries must be discretized.

Advantage: Cheap descretization, some special boundary conditions can be represented very well

Disadvantage: very expensive calculations, heterogenities also expensive, mostly distributed at universities

Finite Difference Method



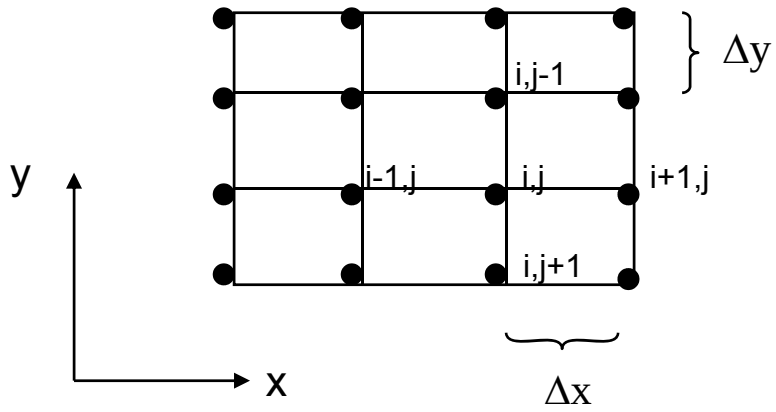
Model domain is subdivided into a uniform grid.
In the nodes (centre or edges of the grid) derivation to time or space are substituted by difference quotient. The resulting simple discrete equation system can be solved very well by computers (specific iteration schemes).

Advantage: easy, fast and accurate, well developed, heterogenities very flexible to represent

Disadvantage: discretization not flexible, many nodes, no local refinements

Finite Differenzen Methode

DGL Zweidimensionale Strömung im homogenen Medium: $$T\left(\frac{\partial^2 h}{\partial x^2}+\frac{\partial^2 h}{\partial y^2}\right)=Q$$



„5-Punkte-Stern“

Differentiationen durch Differenzenquotienten ersetzten:

$$-T_{i,j}\left[\frac{\frac{h_{i+1,j}-h_{i,j}}{\Delta x}-\frac{h_{i,j}-h_{i-1,j}}{\Delta x}}{\Delta x}+\frac{\frac{h_{i,j+1}-h_{i,j}}{\Delta y}-\frac{h_{i,j}-h_{i,j-1}}{\Delta y}}{\Delta y}\right]=Q_{i,j}$$

$Q_{i,j}$ Quellen im Block i,j [m^3/sm^2]

$T_{i,j}$ Transmissivität des Blocks i,j [m^2/s]

Aufstellen dieser Gleichung für jeden Knoten i,j ergibt das Gleichungssystem, das direkt oder iterativ gelöst werden kann. (Iterative Löser: z.B. Jacobi oder SOR)

Convergence of FD Iteration schemes

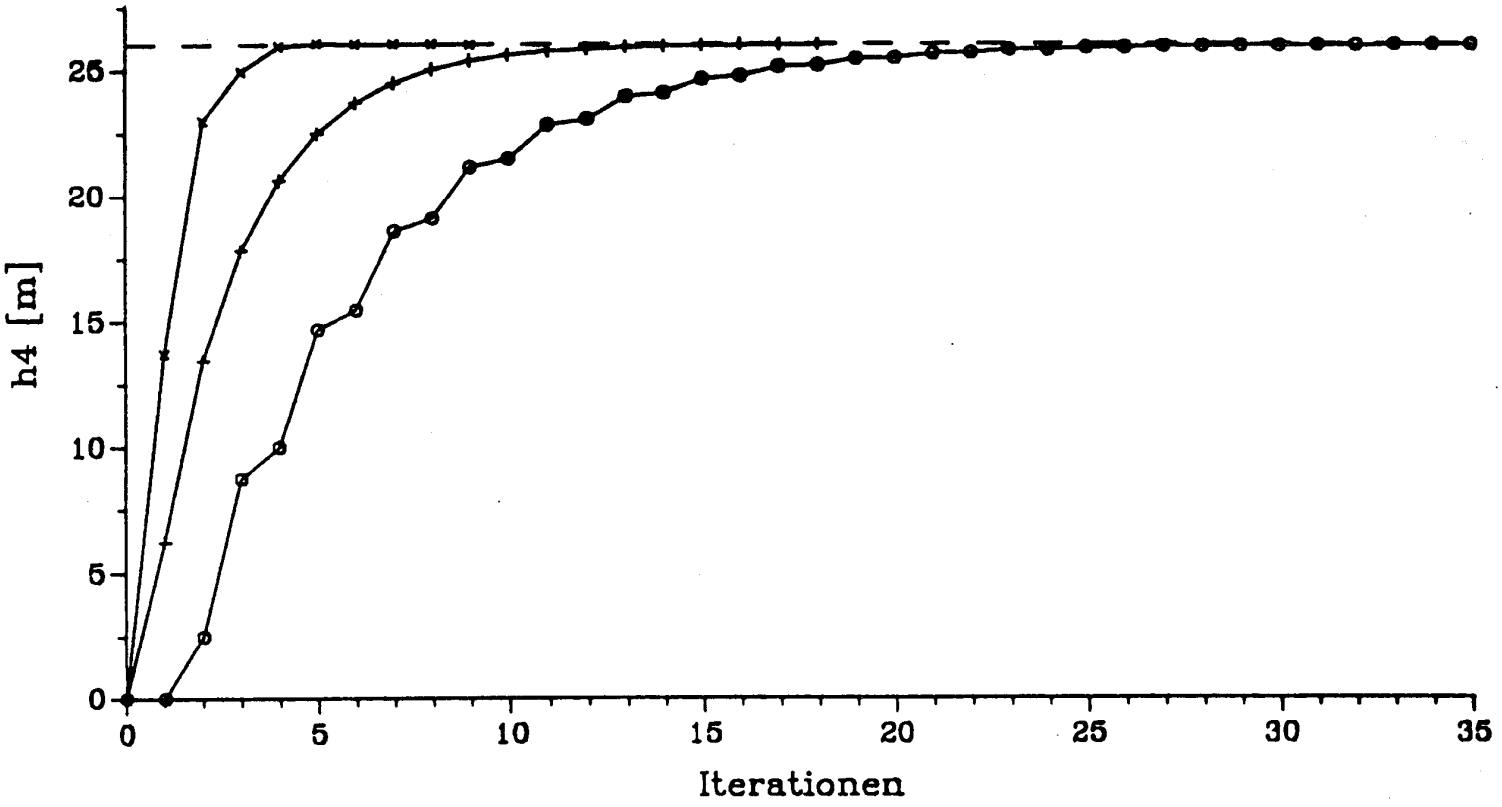


Abb. 14: Konvergenzverhalten unterschiedlicher Iterationsverfahren (o = Jacobi, + = Gauß-Seidel, × = SOR mit $\omega = 1.3$). Dargestellt ist jeweils die Veränderung des Potentials h_4 im Verlaufe der Iteration. Für das SOR-Verfahren wurde der in diesem Fall als optimal anzusehende Wert von $\omega = 1.3$ gewählt, der zu einer sehr schnellen Konvergenz führt ohne über den exakten Wert (unterbrochene Linie) hinauszuschwingen (vgl. Abb. 15).

SOR Iteration for different weighting factors

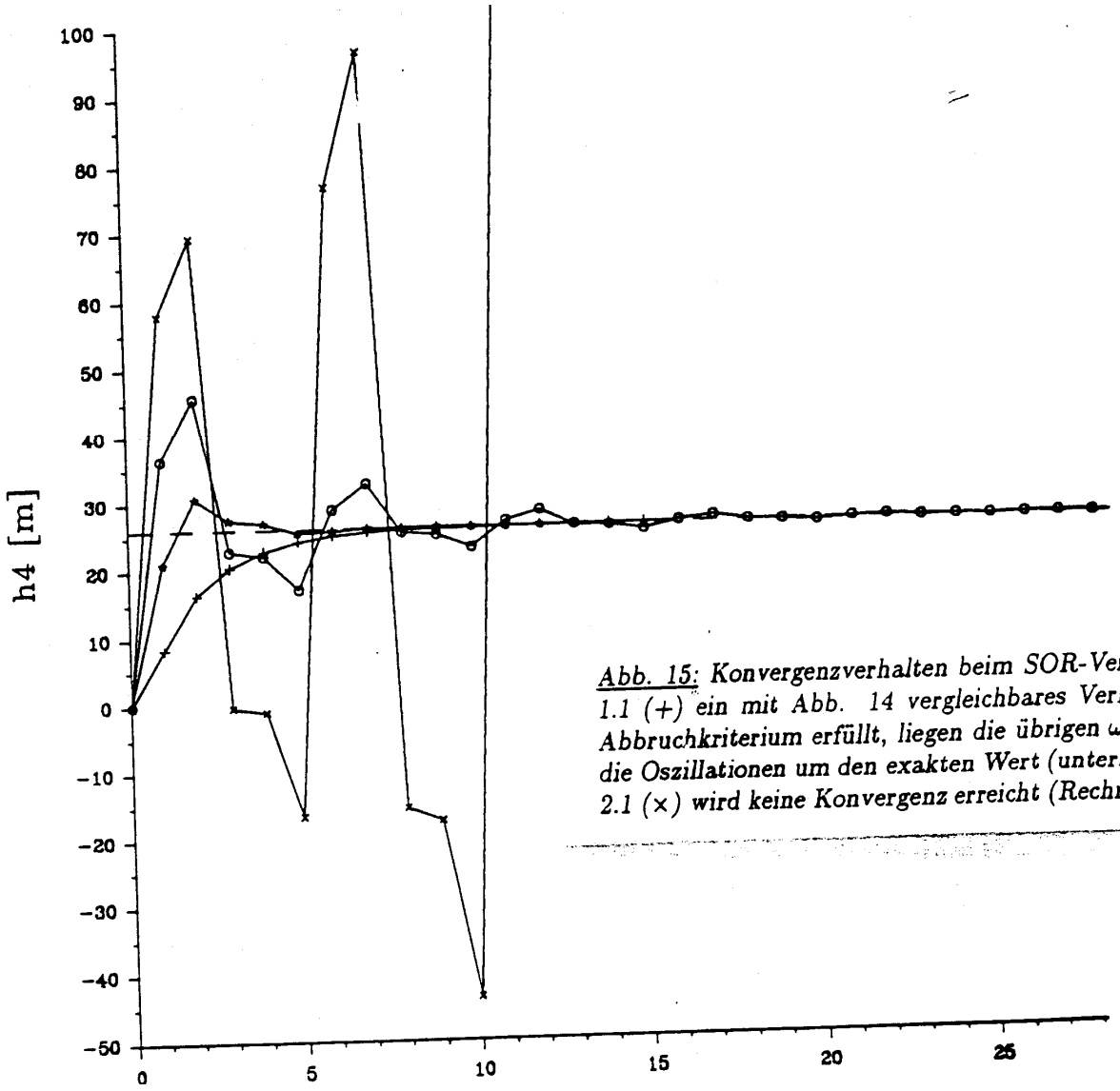
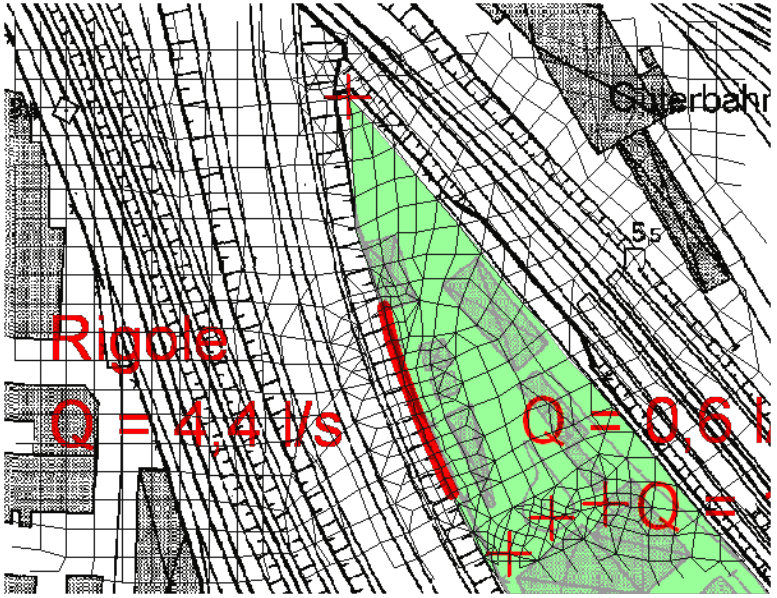


Abb. 15: Konvergenzverhalten beim SOR-Verfahren für unterschiedliche ω-Werte. Währe
1.1 (+) ein mit Abb. 14 vergleichbares Verhalten zeigt, allerdings erst nach 12 Iteratio
Abbruchkriterium erfüllt, liegen die übrigen ω-Werte (⋆ = 1.5, ∘ = 1.8) zu hoch und führe
die Oszillationen um den exakten Wert (unterbrochene Linie) zu schlechteren Ergebnissen. I
2.1 (×) wird keine Konvergenz erreicht (Rechnung wurde nach 11 Iterationsschritten abgeb

Finite Element Method

PDE is transverted into a domain integral equation („weak form“).

Model domain is subdivided into elements.
Within the elements the solution of the weak form is interpolated by shape functions.
Collocations points are the nodes.



Advantage very flexible dicretization, well distributed, well developed

Disadvantage conservation equations are not exactly fulfilled (mass, momentum)

Verfahren FE (1)

Die DGL mit den Randbedingungen stellt die starke mathematische Formulierung dar:

$$\frac{\partial}{\partial x_i}\left(-K_{ij}\frac{\partial}{\partial x_j}h\right)=Q$$

RB 1. Art $h=\bar{h}$

RB 2. Art $q_i n_i=\bar{q}$

RB 3. Art $q_i n_i=f(h)$

Die Schwache Form der DGL kann z.B. durch das Verfahren der Gewichteten Residuen erzeugt werden. Dabei wird der Fehler, der mit der Näherungslösung $\tilde{h}$ gemacht wird, mit einer Wichtungsfunktion W multipliziert und über das Gebiet integriert.
Dieses Integral wird = 0 gesetzt.

$$\int_\Omega\left[W_n\left(\frac{\partial}{\partial x_i}\left(-K_{ij}\frac{\partial}{\partial x_j}\tilde{h}\right)-Q\right)\right]d\Omega=0$$

Bei der Methode der Finiten Elemente wird die Näherungslösung elementweise durch Ansatz- oder Formfunktionen N bestimmt.

$$\tilde{h}(x_i)=\sum_{k=1}^{n}N_k(x_i)\hat{h}_k$$

Durch Normierung der Elemente sind die Ansatzfunktionen stets dieselben. Diese sind so formuliert, dass die Freiwerte $\hat{h}$ den Knotenwerten der Variablen (des Potentials, Drucks oder der Konzentration) entsprechen. Die Ansatzfunktionen müssen die Randbedingungen 1. Art erfüllen.

Verfahren FE (2)

In der Regel werden für die Wichtungsfunktion und für die Interpolationsfunktionen dieselben Funktionen verwendet (Galerkinverfahren).

Diverse Umformungen führen zu der Integralgleichung, die mit Standardgleichungslösern am Rechner gelöst werden kann.

Randbedingung 2. Art

$$\underbrace{\int_{\Omega} \frac{\partial N_n}{\partial x_i}(-K_{ij})\frac{\partial N_k}{\partial x_j} d\Omega}_{\text{Strömungsmatrix}} \hat{h}_k = \underbrace{\int_{\Gamma} N_n q^{in} d\Gamma + \int_{\Omega} N_n Q d\Omega}_{\text{Quellenvektor}} = P_n$$

Vektor der unbekannten Knotenpotentiale

kurz: $H_{nk}\hat{h}_k = P_n$

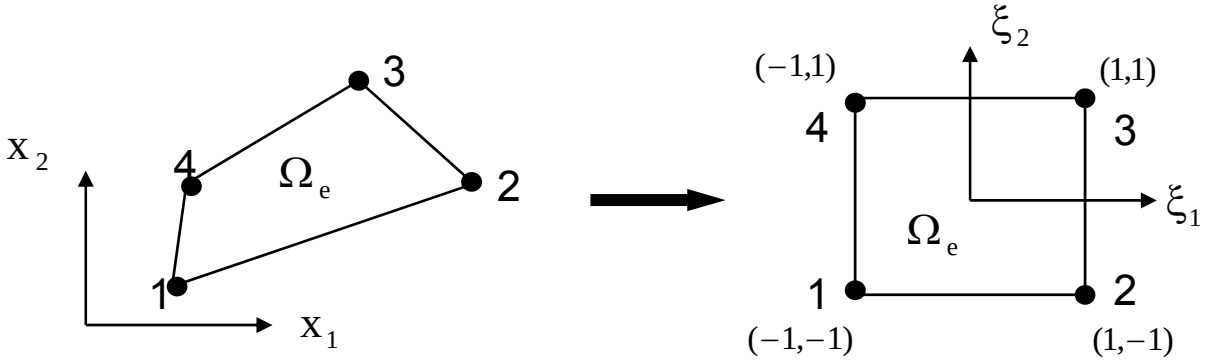
Die Integralgleichung wird für jedes Element aufgestellt und anschließend zu einem Gesamtgleichungssystem assembliert.

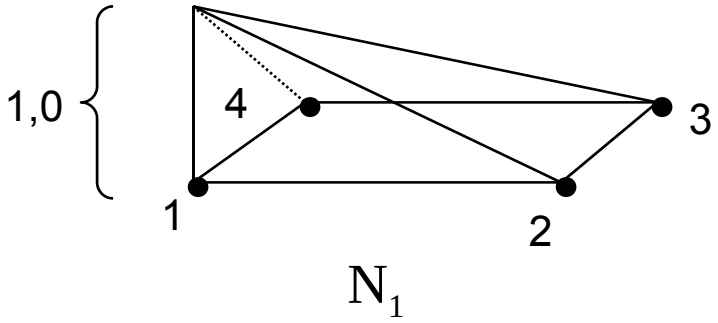
Berechnung der Massenflüsse anschließend an die Berechnung der Potentiale (Nachlauf)

$$q_i = -K_{ij}\frac{\partial}{\partial x_j}\left(N_k(x_i)\hat{h}_k\right)$$

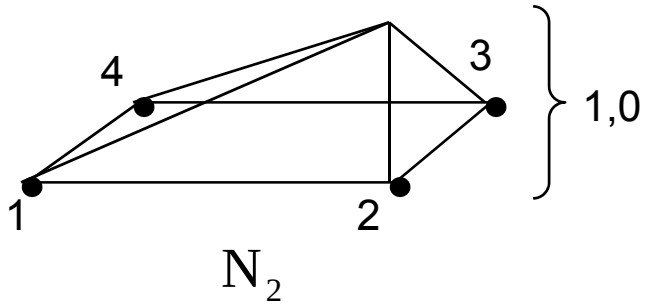
Shape functions

Normalized element coordinates





N_1



N_2

$$N_1 = \frac{1}{4}(1-\xi_1)(1-\xi_2) \qquad N_3 = \frac{1}{4}(1+\xi_1)(1+\xi_2)$$

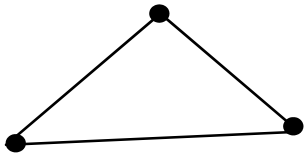
$$N_2 = \frac{1}{4}(1+\xi_1)(1-\xi_2) \qquad N_1 = \frac{1}{4}(1-\xi_1)(1+\xi_2)$$

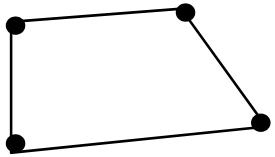
linear shape function
4 node elements

Element Types

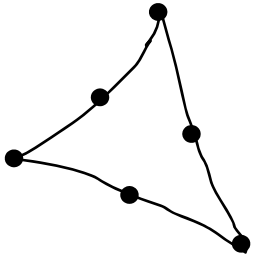
Normally isoparametric elements are used. In this case elements with linear shape functions have linear edges.

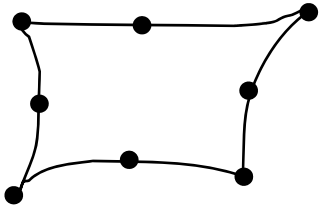
linear 1D element



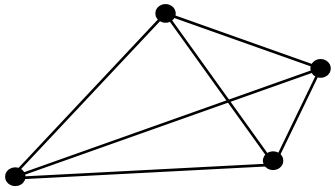


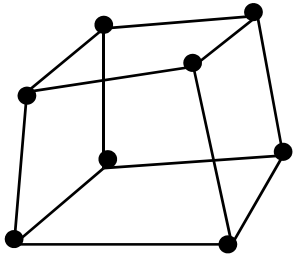
linear 2D elements





quadratic
2D elements





linear 3D elements

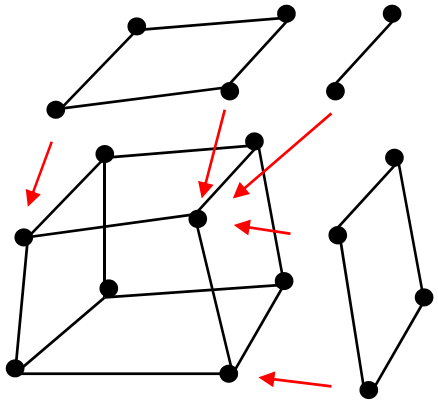
also 5,6 oder 7 nodes possible

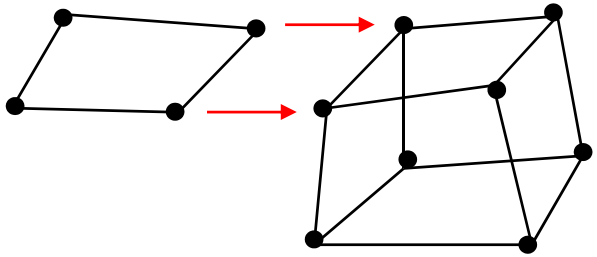
Discretization

Subdivision of domain in nodes and elements is called *discretization.*
The finer the discretization is, the higher the accuracy of numerical approximation.

Production and observation wells, receiving waters, lakes etc. should always be at nodes or element edges.

Elements are connected by nodes. For that reason it is no problem to couple elements of different dimensions (e.g. 1D for flow channels, 2D for fractures, 3D for solid matrix)

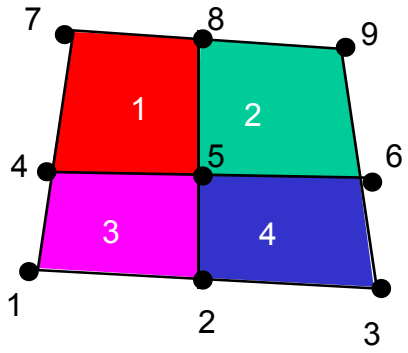




Assembling

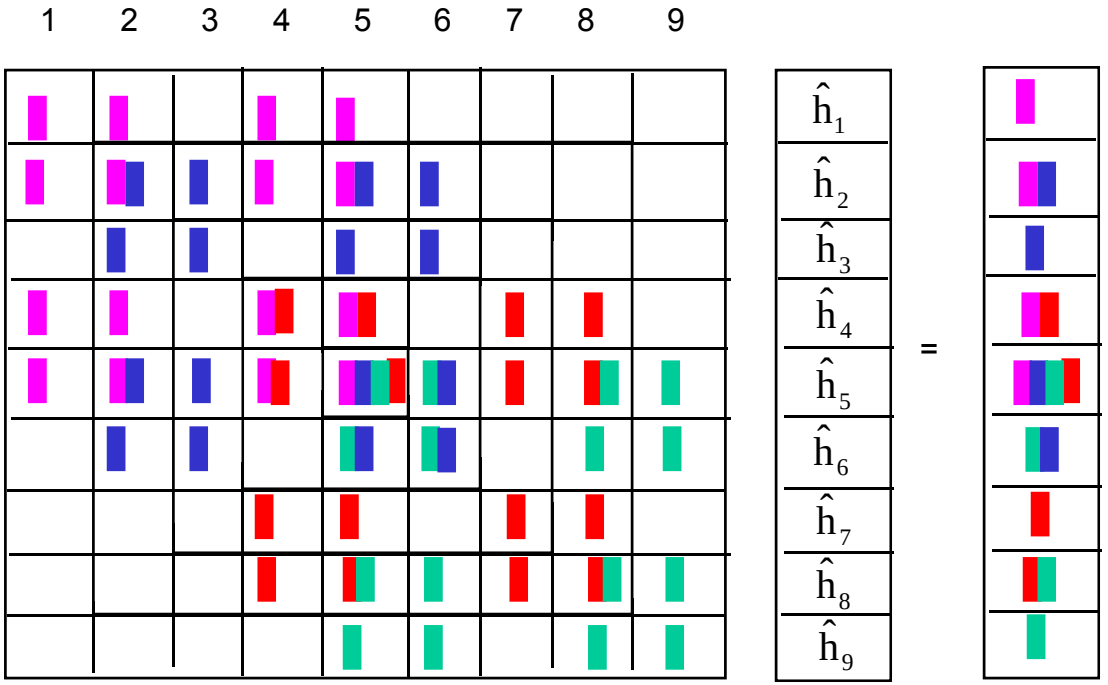
Assembling of element matrices to the global matrices (flow matrix and source vector):

Matrix components of the same node are added.



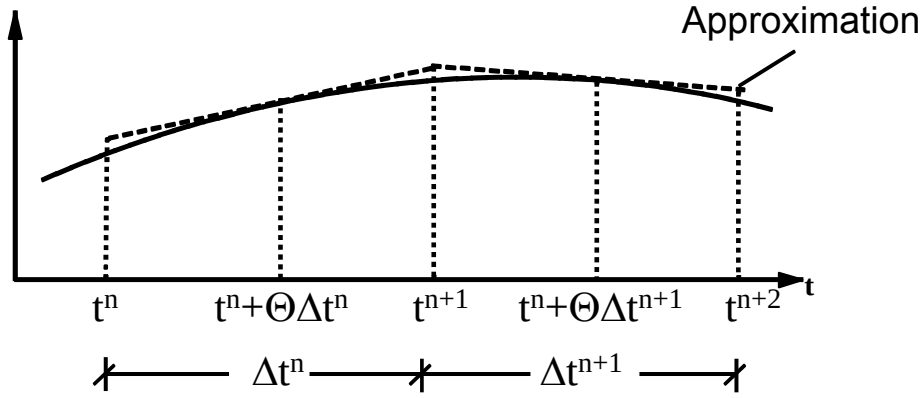
$$H^3_{ij} = \begin{bmatrix} & 1 & 2 & 5 & 4 & \\ 1 & & & & & \\ 2 & & & & & \\ 5 & & & & & \\ 4 & & & & & \end{bmatrix}$$

global degrees of freedom



$$H_{ij}\hat{h}_j = P_i$$

Time discritization



Method	Order	Characteristics
0	explicit	Stability only for very small time steps, high accuracy
1/2	Crank-Nicolson	Stable
2/3	Galerkin	Stable
1	fully implicit	stable, small accuracy

Time Discretization

Transient flow equation, discretized in space

$$\underline{S}\frac{\partial \underline{h}(t)}{\partial t} + \underline{H}\,\underline{h}(t) = \underline{P}(t)$$

t time coordinate
$\underline{h}$ node potential head, time dependent
$\underline{S}$ storage matrix
$\underline{H}$ flow matrix
$\underline{P}$ source vector

time discretization with finite differences

$$h(t) = \Theta h^{t+1} + (1-\Theta)h^{t}$$

$$\frac{\partial h(t)}{\partial t} = \frac{1}{\Delta t}(h^{t+1} - h^{t})$$

Θ collocation point

leads to

$$\frac{1}{\Delta t}\underline{S}(\underline{h}^{t+1} - \underline{h}^{t}) + \underline{H}(\Theta\underline{h}^{t+1} + (1-\Theta)\underline{h}^{t}) = \Theta\underline{P}^{t+1} + (1-\Theta)\underline{P}^{t}$$

known terms to right hand side:

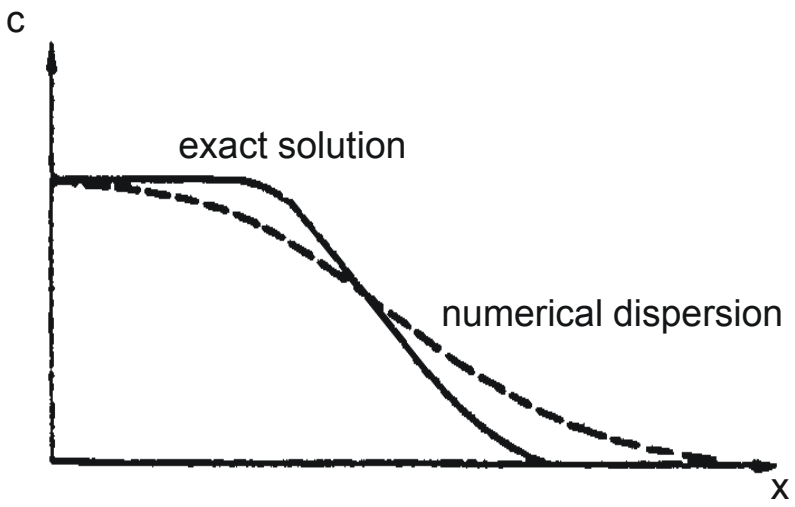
$$\left(\frac{1}{\Delta t}\underline{S} + \Theta\underline{H}\right)\underline{h}^{t+1} = \Theta\underline{P}^{t+1} + (1-\Theta)\underline{P}^{t} + \left(\frac{1}{\Delta t}\underline{S} - (1-\Theta)\underline{H}\right)\underline{h}^{t}$$

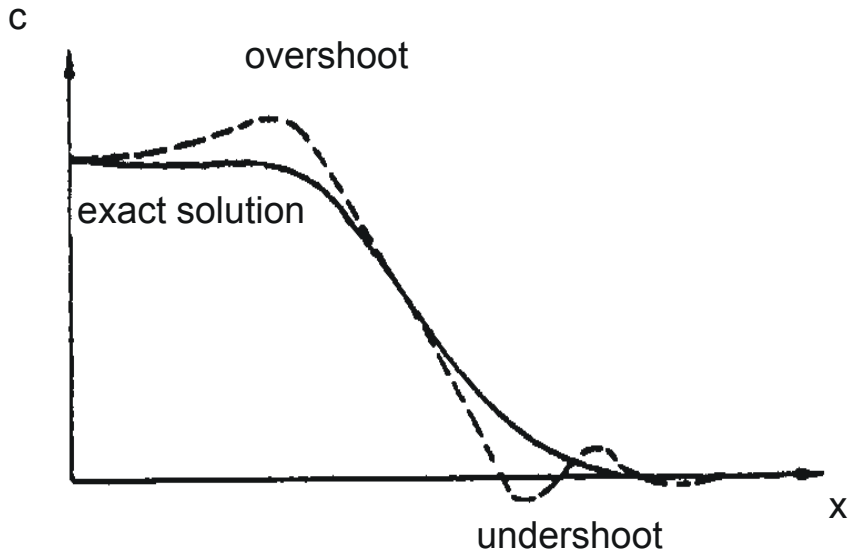
Algebraic equation for transient flow

Stability of Numerical Solution

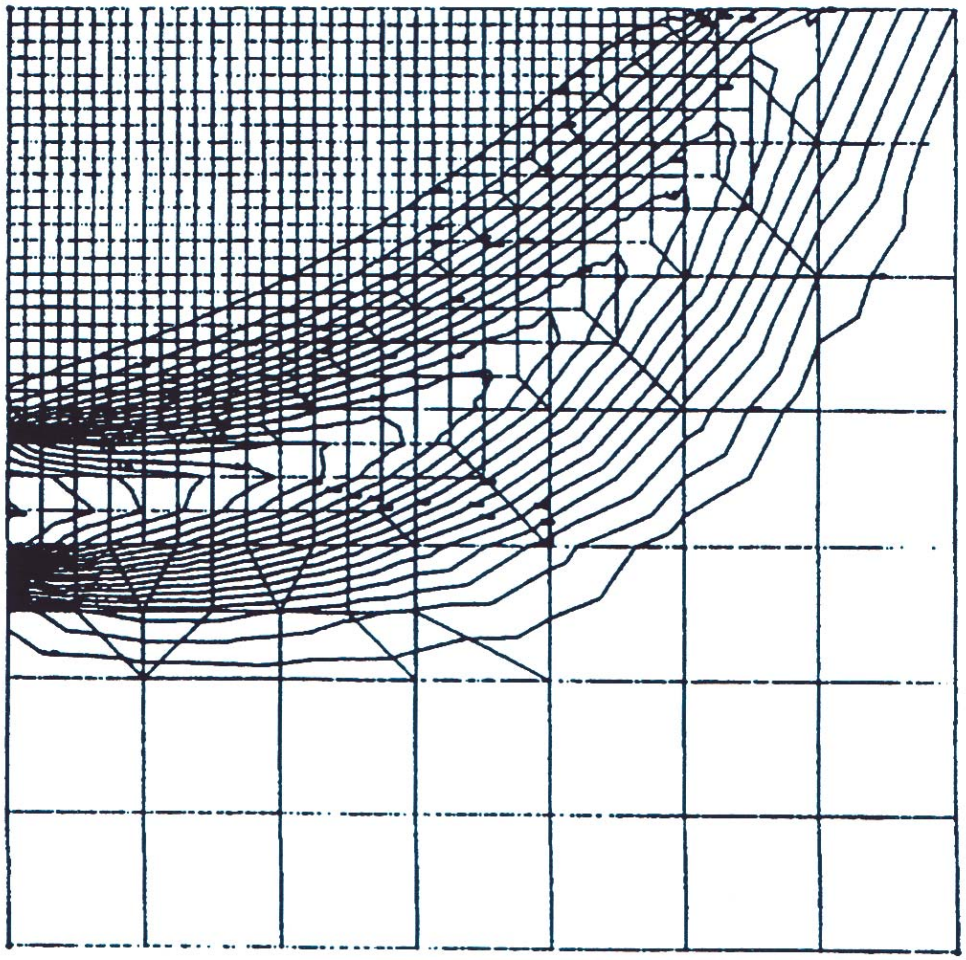
Transport Approximation

Numerical Problems

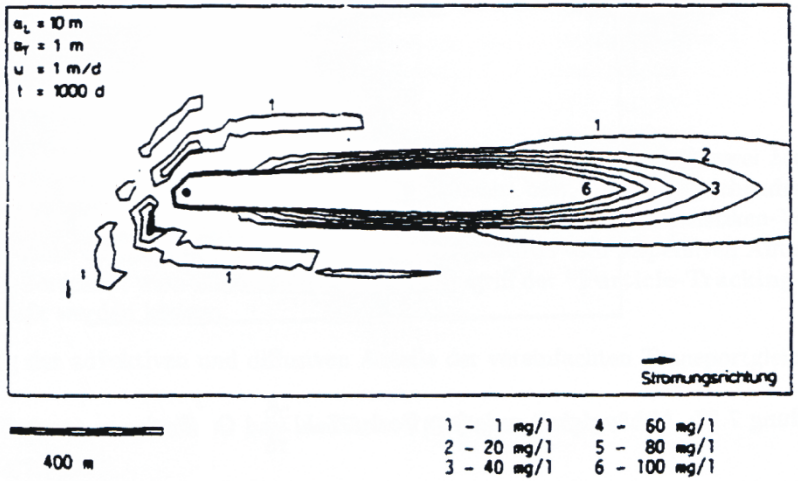




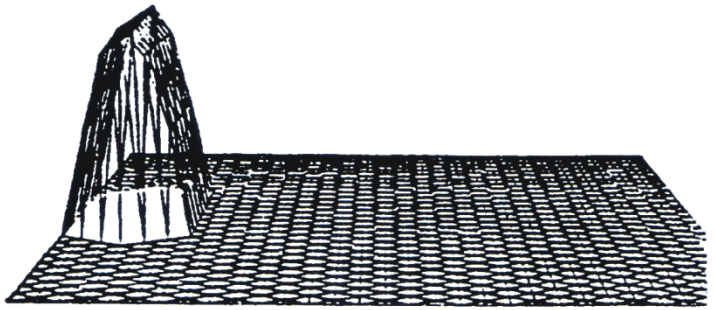
Influence of Discretization to Numerical Dispersion



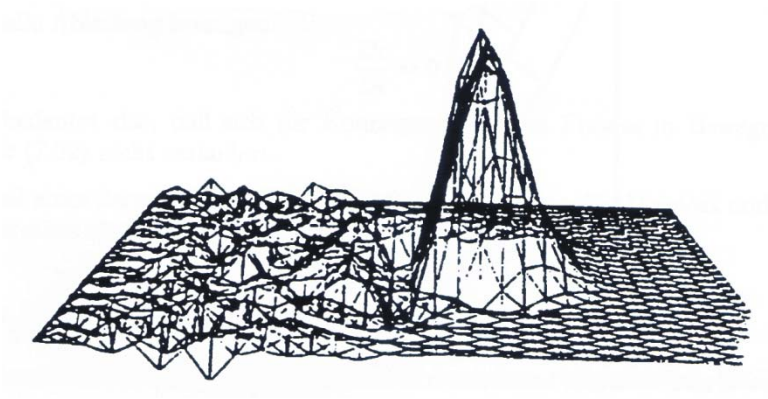
Oscillations



concentrations (isolines)



initial concentration



concentration with oszillations

Stability Criteria for Transport

Peclet number

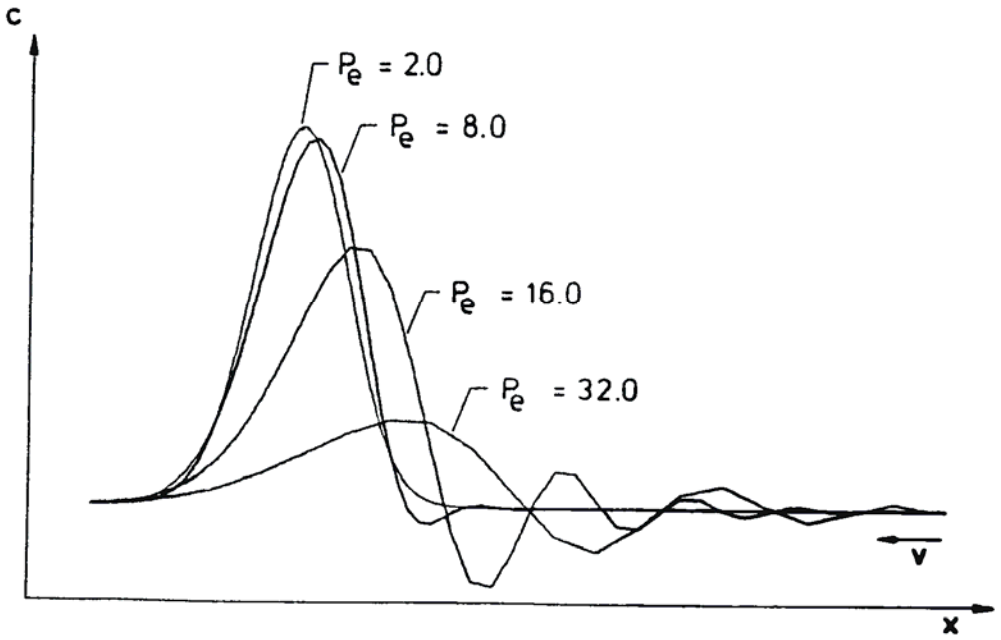
Peclet number is the ratio of advective to dispersive transport. Numerical stability can be measured by the Peclet number.

For Pe>1 advection is dominant => Numerical Oscillations can occur at the propagation front of the substance. The higher the concentration gradient is, the more numerical problems occur.

$$Pe = \frac{v\Delta l}{D}$$

- D Diffusion coefficient
- v distance velocity
- Δl charakteristical element length

Good results can be expected for Pe < 2



Stability Criteria Transport

Courant Criteria

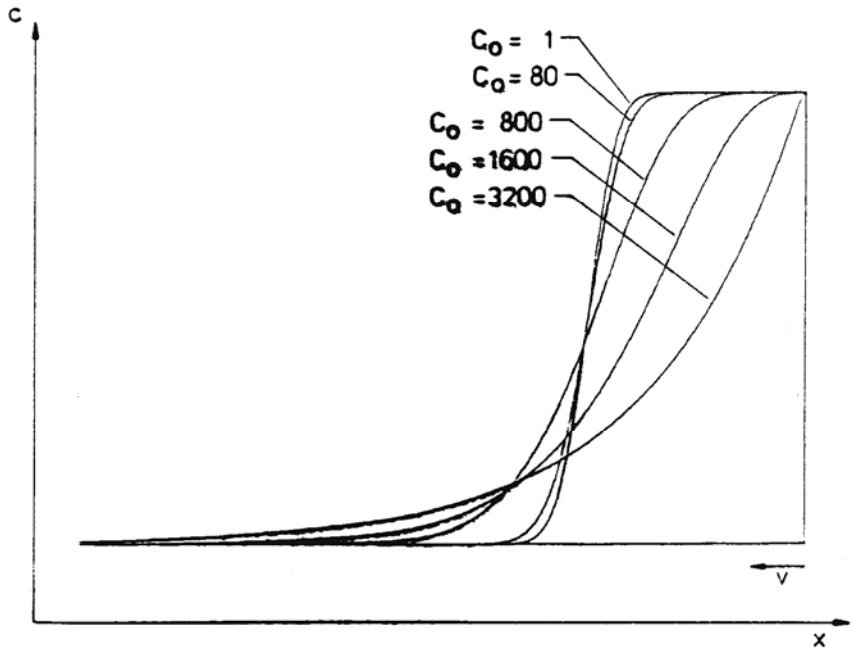
The Courant criteria measures the ratio of time discretization to space discretization.
If a particle moves more than an element length during a time step numerical disperison occurs. The propagation front is approximated too soft.

$$Co = \frac{v\Delta t}{\Delta l}$$

Δt time step width

v distance velocity

Δl characteristical element length



Good results can be expected for Co $\leq$1

Stable Transport Simulation

Discretization

Consider stability criteria in the area of substance plume

→ local refinements

time step width

stable methods

Upwind Methods
(Unsymmetrical Weighting of advektive term)

Splitting Methods
(Advection and Diffusion/Dispersion are solved separatly)

Euler-Lagrange-Methods
(Particle Tracking)

...combined with standard FE or FD for flow simulation

Flow and Transport Simulation

- Transport simulation needs flow velocity

  $\Rightarrow$ Each transport simulation need flow simulation

- Influence of transport on groundwater flow by density and viscosity

  $\rightarrow$ If density or/and viscosity are influences by the transport processes flow and transport simulation is coupled

otherwise flow simulation is independent of transport simulation

Software

MODFLOW (flow), **MT3D** (transport), **RT3D** (reactive transport)

flow: Finite Differences (FD), Transport: FD, Particle Trecking, FV

www.modflow.com Mainprocessing is Freeware (supported by US Government), Pre- and Postprocessing commercial (PMWIN, Visual Modflow, GMS, Groundwater Vistas)

most common groundwater software

SPRING Finite Element Method

www.deltah.de incl. Pre- und Postprocessing, commercial