

### Groundwater modeling: flow simulations

### A. Dassargues

References:

Dassargues A., 2018. Hydrogeology: groundwater science and engineering, 472p. Taylor & Francis CRC press (chapters 4, 12 & 13) Dassargues A. 2020. Hydrogéologie appliquée: science et ingénierie des eaux souterraines, 512p. Dunod (chapitres 4, 2 et 13)

#### Groundwater modeling: flow simulation

- Groundwater flow equations
  - REV concept
  - Potentiometric/piezometric head
  - Porosities, hydraulic conductivty, Darcy's law, transmissivity
  - Steady state equations
  - Transient equations
  - Extending to partially saturated flow
- Flow Boundary Conditions
  - Dirichlet BC's
  - Neumann BC's
  - Cauchy BC's
- Introduction to solving methods
  - Finite Difference method
  - Time integrations schemas
  - Finite Difference method (FD): practical recommendations
  - Finite Element method: summary
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- References



### Assumptions and REV concept



REV is the volume of geological medium considered as representative for quantification of the value of the different properties (by averaged, equivalent values)

> large enough to be relevant with regard to the studied problem (avoid microscopic scale for a real case study)

> small enough for avoiding too smoothed values that will corrupt our description of the processes



... this REV concept implicitly implies that the medium is considered as continuous (and porous)

- the REV depends on the kind of problem being studied and the study objectives
- the REV is used for groundwater flow and solute transport ... but also in all other fields where a quantification is needed for properties of the geological medium

(de Marsily 1986, Dagan 1989, Bear & Verruijt 1987)

# Assumptions, REV concept and scale



parameter values can be quite different in function of the considered scale

(Dassargues & Monjoie 1993, Dassargues 2018 and 2020, Hoffmann et al. 2021)

### **Hydrostatic**



### ... the potential energy is expressed usually in 'water head' or hydraulic head or piezometric head:



### Water pressure vs piezometric head



 $\rightarrow$  ... a direct link between hydraulic/piezometric head h and water pressure p:  $p - (h - z) \circ a$ 



for groundwater flow problems, the main variable is the piezometric head or the water pressure



piezometric heads can be compared only if groundwater has everywhere the same temperature and the same salt content



*if it is not the case, ... density will vary ... and to a same water pressure correspond different piezometric heads (of groundwater with different salt content) Rmq: if density effect (salwater) is considered work with pressure or with 'equivalent* 

freshwater piezometric heads' 6 6 6 (Carabin and Dassarques 1999)





**T** 7

### **Porosity**

... two components in the total porosity:

 $\rightarrow$  cinematic porosity  $n_c$ 

retention capacity' or 'specific retention')  $S_r$ 

$$n_c + S_r = n$$
 with  $n_c = \frac{V_m}{V_t}$   $S_r = \frac{V_{im}}{V_t}$ 

the cinematic porosity is difficult to be measured in practice (... after which duration ? ... at which pressure ? ... )

drainage porosity = effective porosity  $\mathcal{N}_e \cong \mathcal{N}_c$ corresponding to the drainable water by gravity (also called mobile water or free water) .... also called = "specific yield"  $S_v$ 

### **Porosity and granular analysis**





(Eckis 1934, Castany 1963)

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### Hydraulic conductivity and Darcy's law

V

... experimental law

quantity of water per time unit through a porous medium:

$$Q = K.A.\frac{\Delta h}{L}$$



permeability coefficient, hydraulic conductivity, water permeability (by abuse of language: permeability) of the porous medium (m/s)

... specific flux or flow rate (specific discharge):

$$q = \frac{Q}{A}$$

*in m<sup>3</sup>/(m<sup>2</sup>.s) ... in m/s* 

### Hydraulic conductivity and Darcy's law

the actual groundwater flow section is :

This specific discharge is often called 'Darcy's velocity' ... it is only a flow rate Q divided by a surface A

this surface is not the groundwater flow section

... to obtain a mean (averaged/equivalent on the REV)

groundwater velocity :

$$v_e = \frac{q}{n_e} = \frac{K}{n_e} \frac{\Delta h}{L}$$

m/s

*'advection velocity'* (effective velocity)

 $A.n_{\rho}$ 

### ...about mobile water porosities



the 'mobile water porosity' to be considered for groundwater flow is typically higher than the 'mobile water porosity' acting in solute transport processes (Payne et al. 2008, Hadley and Newell, 2014)

#### Box 8.1 About effective transport porosity

Effective transport porosity is in reality very dependent on what we define as mobile and immobile groundwater in the representative volume of geological medium. For many contamination problems and associated risk assessments, it is very important to predict the first arrival time of solute contaminant at a "target." This is the case, for example, for protection zone delineation around a pumping well, for security assessment of waste disposal, for assessment of risk created by industrial contamination hazards, and for groundwater vulnerability mapping. To be conservative (i.e., on the security side) with regards to most practical applications where solute transport is calculated, one should choose to define the effective porosity relevant to solute advection as a relatively small part of the total porosity. This is especially true and important if the geological medium is known as a "dual" porosity medium or is highly heterogeneous at the micro- and macroscales. If the Darcy flux (i.e., specific discharge, see Chapter 4, Section 4.4) would be divided by the total porosity n, this would produce a kind of averaged velocity between the mobile and immobile groundwater in the medium which can be highly misleading (i.e., leading to underestimated velocities). However, some can argue that this could be partially and artificially compensated or corrected by considering larger values of the longitudinal dispersivity.

useful
 porosity for
 solute
 transport is
 'effective
 transport
 porosity'
 < drainage</li>
 porosity



### **Generalisation of the Darcy's law in 3D**



hydraulic conductivity and intrinsic permeability described by

tensors:  $\mathbf{K} = \begin{bmatrix} K_{xx} & K_{xy} & K_{xz} \\ K_{yx} & K_{yy} & K_{yz} \\ K_{zx} & K_{zy} & K_{zz} \end{bmatrix} \quad \text{and} \quad \mathbf{K} = \mathbf{k}\rho g/\mu$ 

> elevation of the considered point (with regards to the reference datum)

**grad** 
$$h = \nabla h = \left(\frac{\partial h}{\partial x}, \frac{\partial h}{\partial y}, \frac{\partial h}{\partial z}\right)$$







aquifer at the concerned point

conductivity on the vertical of the concerned point









### **Equation in transient conditions**





### Specific storage coefficient



... often, the influence of the water compressibility and the solid grain compressibility can be neglected with regards to the volume compressibility of the porous medium (as a whole)

$$\longrightarrow S_s = \rho g \alpha$$

... this link between the volume compressibility and the specific storage coefficient is showing clearly the direct coupling between saturated transient groundwater flow and geomechanical behaviour in compressible porous media

the volume compressibility is dependent on

- *effective stress variation*
- the effective preconsolidation stress of the porous medium
  Rmg: So is actually variable as it depends on compressibility that is

*Rmq:*  $S_s$  is actually variable as it depends on compressibility that is dependent on the effective stress state that is dependent on the water *pressure,...* (Dassargues et al. 1991 and 1993, Dassargues 1995, 1997, 1998)

### **Equation in transient conditions**



Storage coefficient = water volume  $(m^3)$  stored or drained per aquifer surface unit  $(m^2)$  for a unit variation of piezometric head (m)



the most important part of the storage is due to saturation/drainage of the porous medium

(Dassargues 1995b, 2018, 2020)

### Storage coefficient





### 2D groundwater flow equations in transient conditions (horizontal flow)



$$\nabla \cdot (\mathbf{T} \cdot \nabla h) + q'' = S \frac{\partial h}{\partial t}$$
terms are in m/s
$$\frac{\partial}{\partial x_i} \left( T_{ij} \frac{\partial h}{\partial x_j} \right) + q''_i = S \frac{\partial h}{\partial t}$$
in indicial notation
$$\frac{\partial}{\partial x} \left( T_{xx} \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left( T_{yy} \frac{\partial h}{\partial y} \right) + q'' = S \frac{\partial h}{\partial t}$$
principal anisotropy directions aligned
with the selected coordinate system
$$\frac{\mathbf{unconfined aquifer}}{\mathbf{unconfined aquifer}}$$

$$\nabla \cdot (\mathbf{T}(h) \cdot \nabla h) + q'' = n_e \frac{\partial h}{\partial t} = S_y \frac{\partial h}{\partial t}$$
terms are in m/s
$$\frac{\partial}{\partial x_i} \left( T_{ij} \frac{\partial h}{\partial x_j} \right) + q''_i = n_e \frac{\partial h}{\partial t} = S_y \frac{\partial h}{\partial t}$$
in indicial notation
$$\frac{\partial}{\partial x_i} \left( T_{xx} \frac{\partial h}{\partial x_j} \right) + q''_i = n_e \frac{\partial h}{\partial t} = S_y \frac{\partial h}{\partial t}$$
in indicial notation

system

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### Particular case: 2D horizontal confined flow



vertical integration of the 3D equation on the thickness of the confined aquifer

$$\frac{\partial}{\partial x} \left( T_{xx} \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left( T_{yy} \frac{\partial h}{\partial y} \right) = S \frac{\partial h}{\partial t} - R + L$$

where T: transmissivity  $[L^2 T^{-1}]$ ,  $K \times$  thickness S: storage coefficient [-],  $S_s \times$  thickness R: recharge rate  $[L^3 L^{-2} T^{-1}] = [L T^{-1}]$  L: leakance  $[L T^{-1}]$ Recharge (R)  $\downarrow$ Thickness (b)

### Particular case: 2D horizontal confined flow



### ... leakance calculation for a quasi 3D approach

Multi-aquifer system **a** Leakance (vertical flow) through the aquitard Darcy's law  $L = -\frac{K_z(h_s - h)}{h_s}$ 

où K'<sub>z</sub> : vertical hydraulic conductivity of the aquitard
 b' : aquitard thickness
 h<sub>s</sub> : surperfical aquifer piezometric head

h : main aquifer piezometric head (main variable)



# Groundwater flow equations including the partially saturated zone

$$\nabla \cdot \rho \big[ \mathbf{K}(h_p) \cdot \nabla h_p + \mathbf{K}(h_p) \cdot \nabla z \big] + \rho q' = \rho C(h_p) \frac{\partial h_p}{\partial t}$$

(Celia et al. 1990, Dassargues 1997)

with water pressure head as main variable

terms are kg/(m<sup>3</sup>s)

 $\sim 1$ 

$$\nabla \cdot \rho \big[ \mathbf{K}(\theta) \cdot \nabla h_p + \mathbf{K}(\theta) \cdot \nabla z \big] + \rho q' = \rho \frac{\partial \theta}{\partial t} \quad \text{(Richards 1931)}$$

in a mixed way as a function of the water content and the pressure head

needs relations between

- $\theta$  and  $h_p$
- θ and Κ́

. . .

... van Genuchten relations and others

$$p_c/\rho g = -h_p = -p/\rho g = z - h$$

### Flow Boundary Conditions



- Dirichlet conditions: prescribed piezometric head
   Neumann conditions: prescribed flux
- Cauchy or mixed conditions: flux depending on piezometric head

## Practical examples where groundwater flow BCs are discussed on various practical cases are available from the experience of the author and researchers from his team in the following references:

Dassargues et al. 1988, Dassargues 1991, Stefanescu & Dassargues 1996, Dassargues 1997, Carabin & Dassargues 2000, Brouyère et al. 2004, Peeters et al. 2004, Rojas & Dassargues 2007, Rocha et al. 2007, Rojas et al. 2008, Jusseret et al. 2009, Goderniaux et al. 2009, Brouyère et al. 2009, Rojas et al. 2010, Wildemeersch et al. 2010, Orban et al. 2010, Goderniaux et al. 2011, Wildemeersch et al. 2014, César et al. 2014, Pujades et al. 2016)





### Prescribed piezometric head

(Dirichlet condition)

Prescribed piezometric head on the concerned boundary:

$$h(x, y, z, t) = f'(x, y, z, t)$$

*f*' can vary in space and time (one value per node and per time step)



a flux will be computed per concerned node



### Flow BC's



### Prescribed flux (Neumann condition)

The first derivative of the piezometric head is prescribed on the concerned boundary:

$$\nabla h \cdot \mathbf{n} = \frac{\partial h}{\partial n}(x, y, z, t) = f''(x, y, z, t)$$

f" piezometric gradient normal to the concerned boundary, its value can vary in space and time (one value per concerned node and per time step) Applying the Darcy's law, it is a way of prescribing the water flux through the boundary:

$$K \frac{\partial h}{\partial n}(x, y, z, t) = q''(x, y, z, t)$$
  
q'' : precribed flux through the boundary (m/s)

• particular case: 
$$f''=0$$

### **Flow BC's** Prescribed flux (Neumann condition)





(Dassargues, 2018)

### Flow BC's Prescribed flux (Neumann condition)





### Flow BC's



### Flux depending on the piezometric head (mixed condition or Cauchy condition)

A combination (linear relation) of the piezometric head and its first derivative is prescribed on the boundary:

$$a.\frac{\partial h}{\partial n}(x, y, z, t) + b.h(x, y, z, t) = f'''(x, y, z, t)$$

*f*'''can vary in space and in time (one value per concerned node and per time step)

- interactions between surface water bodies and groundwater
  - interactions between different aquifers

### Flow BC's Flux depending on the piezometric head (mixed condition or Cauchy condition)



### Flow BC's Flux depending on the piezometric head (mixed condition or Cauchy condition)





prescribing an 'external head' (i.e. not on the true boundary but outside the modelled zone) so that a groundwater flux across the boundary is computed from the difference between this 'external head' and the piezometric head on the model boundary using a given conductance

### **Flow BC's** Flux depending on the piezometric head (mixed condition or Cauchy condition)





represent an evapotranspiration flux leaving the model but dependent on the 'depth to water' (i.e. the land surface elevation minus piezometric head). An extinction depth  $d_{ext}$  corresponding to a critical head  $h_{crit}$  can be defined so that EvT occurs only if the water table is higher

#### Solving a gw flow problem with a Finite **Difference** schema ⊾h(x)

Simple case...

Assumptions:

- steady state  $\longrightarrow \frac{\partial h}{\partial t} = 0$
- no infiltration, no sink/source term
- homogeneity of the medium

2D problem  $\implies I = 0 \quad q = 0$  $\longrightarrow T = Cst$ 



GW flow equation in steady state

$$\implies \frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} = 0$$



### Solving a gw flow problem with a FD schema



Simple case...

Definition of a partial derivative of a function h(x)of the variable x $\frac{\partial h}{\partial x} = \lim_{\Lambda x \to 0} \left( \frac{h(x + \Delta x) - h(x)}{\Lambda x} \right)$ 



spatial discretisation with a grid

 the nodes are the central points of rectangular cells ('Block Centered Finite Difference method' = BCFD)

- the cells are homogeneous ... the continuous variation of the variable is replaced by a discrete variable defined at the central points of the cells
- the approximation of the differential equation is better as the cells are small

### Solving a gw flow problem with a FD schema



Simple case...

#### j columns



the nodes are numbered sequentially, index i, j and piezometric head values  $h_{ij}$ are attributed

### Solving a gw flow problem with a FD schema Simple case...



Taylor series for a continuous function h(x) $h(x + \Delta x) = h(x) + \Delta x. \frac{\partial h(x)}{\partial x} + \frac{(\Delta x)^2}{2!} \cdot \frac{\partial^2 h(x)}{\partial x^2} + \frac{(\Delta x)^3}{3!} \cdot \frac{\partial^3 h(x)}{\partial x^3} + \dots + \frac{(\Delta x)^n}{n!} \cdot \frac{\partial^n h(x)}{\partial x^n}$ ... for  $h_{ii}$  and the x direction: ... terms of the 3<sup>rd</sup> order and more  $h_{i+1j} = h_{ij} + (x_{i+1} - x_i) \cdot \frac{\partial h}{\partial x} + \frac{(x_{i+1} - x_i)^2}{2} \cdot \frac{\partial^2 h}{\partial x^2} \quad \text{are neglected}$  $h_{i-1,j} = h_{ij} + (x_{i-1} - x_i) \cdot \frac{\partial h}{\partial x} + \frac{(x_{i-1} - x_i)^2}{2} \cdot \frac{\partial^2 h}{\partial x^2} \quad \dots \text{ for } \Delta x < 0$  $\frac{h_{i+1j} - h_{ij}}{(x_{i+1} - x_i)} = \frac{\partial h}{\partial x} + \frac{(x_{i+1} - x_i)}{2} \frac{\partial^2 h}{\partial x^2} \quad \text{and} \quad \frac{h_{i-1j} - h_{ij}}{(x_{i+1} - x_i)} = \frac{\partial h}{\partial x} + \frac{(x_{i-1} - x_i)}{2} \frac{\partial^2 h}{\partial x^2}$  $\frac{(h_{i+1j} - h_{ij})}{(x_{i+1} - x_{i})} + \frac{(h_{i-1j} - h_{ij})}{(x_{i} - x_{i-1})} = \frac{1}{2}(x_{i+1} - x_{i-1}) \cdot \frac{\partial^2 h}{\partial x^2}$ 37

### Solving a gw flow problem with a FD schema Simple case...



$$\frac{\partial^2 h}{\partial x^2} = \frac{2}{(x_{i+1} - x_{i-1})} \cdot \left\{ \frac{h_{i+1j}}{(x_{i+1} - x_i)} - \left( \frac{1}{(x_{i+1} - x_i)} + \frac{1}{(x_i - x_{i-1})} \right) \cdot h_{ij} + \frac{h_{i-1j}}{(x_i - x_{i-1})} \right\}$$

*if* 
$$(x_{i-1} - x_i) = \Delta x = (x_{i+1} - x_i)$$



if 
$$\Delta x = \Delta y = \Delta m = Cst$$
  
 $T \cdot \left(\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2}\right) = \frac{T}{(\Delta m)^2} \cdot \left(h_{i+1j} + h_{i-1j} + h_{ij+1} + h_{ij-1} - 4h_{ij}\right) = 0$ 

$$h_{ij} = \frac{1}{4} \cdot (h_{i+1j} + h_{i-1j} + h_{ij+1} + h_{ij-1})$$



### Introduction to solving methods: FD

1D spatial approximation of the gradient by a finite difference:

Forward FD 
$$\frac{\partial h}{\partial x} \approx \frac{h(x + \Delta x) - h(x)}{\Delta x}$$

Central FD 
$$\frac{\partial h}{\partial x} \approx \frac{h(x + \Delta x) - h(x - \Delta x)}{2\Delta x}$$

$$\frac{\partial^2 h}{\partial x^2} \approx \frac{h_{i+1j} - 2h_{ij} + h_{i-1j}}{(\Delta x)^2}$$

In 2D, with a 2<sup>nd</sup> order accurate FD:

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} \approx \frac{\left(h_{i+1j} + h_{i-1j} + h_{ij+1} + h_{ij-1} - 4h_{ij}\right)}{(\Delta m)^2} = 0$$



### Solving a gw flow problem with a FD schema Generalisation $\begin{array}{c|c} \hline B \\ \hline \bullet E \end{array} \quad \longrightarrow \quad \int_{AB} T_x \frac{\partial h}{\partial x} dy + \int_{BB'} T_y \frac{\partial h}{\partial y} dx +$ $\int_{B'A'} T_x \frac{\partial h}{\partial x} dy + \int_{A'A} T_y \frac{\partial h}{\partial y} dx = Q_C$ Α' •S $T_{xEC}\left(\frac{h_E - h_C}{x_E - x_C}\right)(y_B - y_A) + T_{yNC}\left(\frac{h_N - h_C}{y_N - y_C}\right)(x_B - x_{B'})$ $+T_{xWC}\left(\frac{h_{W}-h_{C}}{x_{W}-x_{C}}\right)(y_{B'}-y_{A'})+T_{ySC}\left(\frac{h_{S}-h_{C}}{y_{S}-y_{C}}\right)(x_{A}-x_{A'})=Q_{C}$

 $\text{ if rectangular cells : } \qquad \Delta x = a \text{ and } \Delta y = b \\ \longrightarrow T_{xEC} \frac{b}{a} (h_E - h_C) + T_{yNC} \frac{a}{b} (h_N - h_C) + T_{xWC} \frac{b}{a} (h_W - h_C) + T_{ySC} \frac{a}{b} (h_S - h_C) = Q_C$ 

### Solving a gw flow problem with a FD schema





$$T_{xEC} \frac{b}{a} (h_E - h_C) + T_{yNC} \frac{a}{b} (h_N - h_C) + T_{xWC} \frac{b}{a} (h_W - h_C) + T_{ySC} \frac{a}{b} (h_S - h_C) = Q_C$$

a ratio of maximum 1/10 for dimensions of the rectangular cells (for good computation conditions)

 $\dots$  if a = b

 $T_{xEC}(h_E - h_C) + T_{yNC}(h_N - h_C) + T_{xWC}(h_W - h_C) + T_{ySC}(h_S - h_C) = Q_C$ 

### Solving a gw flow problem with a FD schema Equivalent values for parameters



... on the basis of the continuity principle

'averaged' or 'equivalent' values between cells



### Solving a gw flow problem with a FD schema Equivalent values for parameters

... for more complex mesh (here nested mesh), the water flux on the boundary :



### Solving a gw flow problem with a FD schema Equivalent values for parameters

$$\int_{AB} T \cdot \left( \frac{\partial h}{\partial x} \cdot n_x + \frac{\partial h}{\partial y} \cdot n_y \right) dS = \frac{|AB| \cdot T_I \cdot T_J}{(|IM| \cdot T_J + |MJ| \cdot T_I)} \cdot (h_J - h_I)$$

… for Control Volume Finite Elements: same principle





### Introduction to solving methods: BCFD





$$T_{eq_{i+}} = \frac{2T_{i+1j}T_{ij}}{T_{ij} + T_{i+1j}}$$



# Introduction to solving methods: time integration scheme



 $\Delta x = \Delta y = \Delta m = Cst$ 



$$h_{ij}(t + \Delta t) = h_{ij}(t) + \frac{Q_{ij}\Delta t}{S} + \frac{T\Delta t}{(\Delta m)^2 S} \Big( h_{i+1j}(t) + h_{i-1j}(t) + h_{ij+1}(t) + h_{ij-1}(t) - 4h_{ij}(t) \Big)$$

- physically: not so accurate T = Cst
  - numerically: stability problem when the time step becomes larger
  - respect a stability criterion

Explicit method  $h_{ij}(t + \Delta t) = h_{ij}(t) + \frac{I \cdot \Delta t}{S} + \frac{T \cdot \Delta t}{(\Delta m)^2 \cdot S} \cdot \left(h_{i+1j}(t) + h_{ij}(t) + h_{ij+1}(t) + h_{ij-1}(t) - 4h_{ij}(t)\right)$ 



<u>10</u>	10	10	10	10	
	10.10 10.075	10.12 10.09	10.10 10.075		Example:
10	10.05 10	10.05 10	10.05 10	10	- squared is
	10.12	10.14	10.12		- initial valu
10	10.09 10.05 10	10.10 10.05 10	10.05 10 10	10	- BC's : h =
	<i>10.10</i> 10.075	<i>10.12</i> 10.09	<i>10.10</i> 10.075		- infiltration
10	10.05 10	10.05 10	10.05 10	10	- S = 0.4 ; 7
					- ⊿t =10 da
<u>10</u>	10	10	10	10	$I.\Delta t$
					=0.05

- squared island
- initial value h = 10 m
- -BC's: h = 10 m
- infiltration: 0.002 m/day
- -S = 0.4;  $T = 100 m^2/day$
- $\Delta t = 10$  days  $\Delta m = 50m$

$$\frac{T.\Delta t}{\left(\Delta m\right)^2.S} = 0.25$$

- ... computation:
- 1<sup>st</sup> time step;
- 2<sup>nd</sup> time step;
- 3<sup>rd</sup> time step;

. . .



# $\frac{\text{Explicit method}}{h_{ij}(t + \Delta t) = h_{ij}(t) + \frac{I.\Delta t}{S} + \frac{T.\Delta t}{(\Delta m)^2.S} \cdot \left(h_{i+1j}(t) + h_{ij}(t) + h_{ij+1}(t) + h_{ij-1}(t) - 4h_{ij}(t)\right)$



Explicit method: stability criterion (example)  $h_{ij}(t + \Delta t) = h_{ij}(t) + \frac{I.\Delta t}{S} + \frac{T.\Delta t}{(\Delta m)^2.S} \cdot \left(h_{i+1j}(t) + h_{i-1j}(t) + h_{ij+1}(t) + h_{ij-1}(t) - 4h_{ij}(t)\right)$ 



... worst case

10 **+** E

10 + E

$$h_{ij}(t) = (10 - \varepsilon)$$

$$h_{ij}(t + \Delta t) = (10 - \varepsilon) + 0 + \alpha(8\varepsilon)$$

$$h_{ij}(t + \Delta t) = 10 + (8\alpha - 1)\varepsilon$$

 $\frac{I.\Delta t}{S} = 0 \qquad \frac{T.\Delta t}{(\Delta m)^2 S} = \alpha$ 

for obtaining the stability :  $(8\alpha - 1)\varepsilon \le \varepsilon$  $\alpha \le 1/4$ 

$$\longrightarrow \frac{T.\Delta t}{(\Delta m)^2.S} = \alpha \le 1/4$$

### Explicit method: stability criterion



the stability of the computations depends on the size of the time step with regards to the size of the grid cells and of the parameters values

stability criterion :

$$\frac{T.\Delta t}{S.(\Delta m)^2} \le \frac{1}{4}$$
$$\frac{T}{S} \cdot \left(\frac{\Delta t}{(\Delta x)^2} + \frac{\Delta t}{(\Delta y)^2}\right) \le \frac{1}{2} \qquad \Delta x \neq \Delta y$$



Additional drawbacks:

- physical propagation of rounding errors
- numerical errors
- Iong CPU time



the unknown cannot be deduced from one equation you need the whole system to be solved

- physically: not so accurate (error increases with time step)
- numerically: unconditional stability
- mathematically: more complex/heavy

(Bear and Cheng 2010)

	Im	olicit	me	thod		
$h_{ij}$	$(t + \Delta$	t).[1+4]	$4.\alpha] = 1$	$h_{ij}(t) + \frac{I}{2}$	$\frac{T \cdot \Delta t}{S}$	
			$+\alpha$ .	$(h_{i+1j}(t +$	$-\Delta t$ ) +	$-h_{i-1j}(t+\Delta t) + h_{ij+1}(t+\Delta t) + h_{ij-1}(t+\Delta t)$
	10	10	10	10	10	even with a $\Delta t = 40$ davs
	10	10.125 10.2 10	10.135 10.2 10	10.125 10.2 10	10	$\frac{I.\Delta t}{T} = 0.2$ $\frac{T.\Delta t}{T} = 1$
	10	10.135 <mark>10.2</mark> 10	10.158 10.2 10	10.135 10.2 10	10	$S$ $(\Delta m)^2.S$
	10	10.125 10.2 10	10.135 10.2 10	10.125 10.2 10	10	<ul> <li> computation:</li> <li>1<sup>st</sup> time step;</li> <li>2<sup>nd</sup> time step;</li> </ul>
	10	10	10	10	10	

*— numerical stability* 

### Implicit method: stability can be proven

$$h_{ij}(t + \Delta t) \cdot [1 + 4.\alpha] = h_{ij}(t) + \frac{I.\Delta t}{S} + \alpha \cdot (h_{i+1j}(t + \Delta t) + h_{i-1j}(t + \Delta t) + h_{ij+1}(t + \Delta t) + h_{ij-1}(t + \Delta t))$$

$$\begin{array}{cccc}
 & I \cdot \Delta t \\
 & I \cdot \varepsilon \\
 & I \cdot \varepsilon$$



### Time integration scheme

### Crank-Nicholson method

- ... at the time  $t + \Delta t/2$ 
  - physically: more accurate
  - numerically: implicit procedure, unconditional stability

### Galerkin method

... at the time  $t + 2\Delta t/3$ 

#### physically: most accurate

numerically: implicit procedure, unconditional stability



### Time integration scheme

 $\theta = 2/3$ 



$$\begin{aligned} \frac{T}{(\Delta m)^2} (h_{i+1j} + h_{i-1j} + h_{ij+1} + h_{ij-1} - 4h_{ij}) + Q_{ij} &= S \frac{h_{ij}(t + \Delta t) - h_{ij}(t)}{\Delta t} \\ \frac{T}{(\Delta m)^2} (1 - \theta) \left( h_{i+1j}(t) + h_{i-1j}(t) + h_{ij+1}(t) + h_{ij-1}(t) - 4h_{ij}(t) \right) \\ &+ \frac{T}{(\Delta m)^2} \theta \left( h_{i+1j}(t + \Delta t) + h_{i-1j}(t + \Delta t) + h_{ij+1}(t + \Delta t) + h_{ij-1}(t + \Delta t) - 4h_{ij}(t + \Delta t) \right) \end{aligned}$$

$\theta = 0$	Full explicit time integration
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- $\theta = 1$  Full implicit time integration
- $\theta = 1/2$  Crank-Nicholson implicit

Galerkin implicit

stability criterion only for explicit schemes  $\theta < 1/2$ 

<sup>55</sup> time integration schemas used in all numerical techniques

# Introduction to solving methods: FD practical recommendations

- an initial field of values for the main unknown variable (piezometric head) needed for initiating the iterative solving
- accuracy increases with the number of cells but portability (i.e. computing efficiency) decreases
- use smaller cells where a steep gradient of the main variable is expected
- spatial discretization: nodes located at pumping wells and observation piezometers
- avoid distances between nodes greater than 1.5 the previous one
- avoid ratios greater than 1/10 for the cell dimensions (bad numerical conditions for solving the system of equations)
- boundaries with a prescribed head should correspond to nodes (central points of the cells, if BCFD)
- boundaries with a prescribed flux should correspond to sides of the cells (where the flux condition is calculated) if BCFD

### Introduction to solving methods: Finite Elements

- discrete elements, unstructured FE mesh
- better for irregular boundaries, spatial variations, and exact locations for stress-factors and observation measurements
- optimized mesh generation to reduce the needed memory space

(refs among others: Narasimhan et al. 1978, Huyakorn and Pinder 1983, Bear and Verruijt 1987, Wang and Anderson 1982, Fitts 2002, Rausch et al. 2005, Bear and Cheng 2010, Anderson et al. 2015, Diersch 2014, Pinder and Celia 2006, Dassargues 2018 and 2020)





### Introduction to solving methods: FE

- the continuous field of the variable (i.e. piezometric head) approximated typically by interpolation functions (here also referred to as basis functions)
- piezometric field described in each finite element by a plane
- the discrete unknowns are the nodal values
- an integral approach expressing the weak formulation (i.e. a variational form integrating the governing partial differential equation of the process with its BCs and initial conditions) for obtaining a global continuum balance statement
- two ways:
  - (1) minimum of a natural variational functional (when it exists)
  - (2) method of weighted residuals (applicable to all types of partial differential equations)





### Introduction to solving methods: FV

- common features with FD and FE
- FD for unstructured grids
- *if triangles: similarities with triangle FE*
- as for FE, FV approximates the main variable using basis functions in the triangular element
- Finite Volume refers to the volume surrounding each node point in a mesh with nodal basis function = 1 only at the considered node and 0 at all others
- conservation law is satisfied locally for a given control volume with respect to its neighboring volumes (similar to FD not to FE)
- balance relies on evaluation of surface integrals on the boundaries (i.e. the conservation must be satisfied across the boundaries of the adjoining control volumes)



(refs among others: Patankar 1980, Baliga and Patankar 1983, Chung 2002, Diersch 2014, Narasimhan and Witherspoon 1976, Rausch et al. 2005, Fletcher 1988, Idelsohn and Onate 1994, Forsyth et al. 1995, Therrien and Sudicky 1996, Pinder and Celia 2006, Therrien et al. 2010)

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