Application of the Cell Method to the Simulation of Unsaturated Flow

S. Straface¹, S. Troisi and V. Gagliardi

Abstract: The present work shows an alternative to the classical methods to solve the Richards' Equation (RE), used to model flow in unsaturated porous media. This alternative is named Cell Method (CM). The CM is based on a preliminary reformulation of the mathematical model in a partially discrete form, which preserves as much as possible the physical and geometrical content of the original problem, and is made possible by the existence and properties of a common mathematical structure of field theories. The goal is to maintain the focus, both in the modelling and discretization steps, on the physics of the problem. The present work derives the discrete formulation of the RE. Because of the nonlinearities involved, RE is often solved using low-order numerical approximation methods, such as Finite Difference (FDM) or Finite Element Methods (FEM). These types of solution methods are used in many of the existing unsaturated flow codes. We show how the CM can be applied in this problem. We have solved a number of test cases, available in literature, to verify the ability of our model to reproduce these results. We have used the Newton-iterative methods which use iterative linear solvers, such as the Bi-CGSTAB. Numerical results, as it is possible to see in the verification exercise section, show the CM to be effective compared with the classical approaches (FDM and FEM) to solve the flow in unsaturated porous media. The procedure presented here is not peculiar to groundwater hydraulics but also applicable in fluid dynamics, solid mechanics, heat conduction and electromagnetism.

1 Introduction

Every time that we construct a physical theory we state the physical laws by means of the more meaningful quantities. Many physical variables exhibit a natural association with geometrical elements [Tonti (2001)]. So there are quantities like temperature, pressure, potential, that

are associated to points. Other quantities are naturally associated to volumes: mass content, heat quantity, internal energy etc. With quantities associated to points it is natural to form the spatial differences: i.e. head difference between two points of an aquifer, pressure difference between two atmosphere points, potential difference between two electrical field point. From these quantities we set the head, pressure and electric potential gradient. With the quantities associated to volumes it is natural to form balance equations: the amount produced in the volume during a time interval is equal to the sum of the outgoing flow of the same quantity across the boundary of the volume during the time interval, and of the quantity stored inside the volume in the same interval. Other physical quantities are naturally associated to surface and time intervals (i.e. flows).

The fundamental laws of physics require geometrical notions for their formulation. So a balance law requires a volume and its bounding surface, a circuital law requires a surface and its bounding line and the notion of the gradient requires two points and the straight line connecting them. Moreover the constitutive equations require the notion of plane and straight line perpendicular to it. The differential formulation of physical laws implies the elimination of geometry by the process of forming the densities of global variables and of performing the limit process to obtain field functions. Differential equations are relations between field functions. The geometrical content is later reconstructed, in order to solve the equations numerically by the integration process. The purpose of this work is to show it is possible to obtain a direct discrete formulation of Richards' equation governing the flow in a unsaturated porous medium, avoiding the passage to the differential formulation and resorting to the use of absolute variables, which allow the physical laws to be preserved in their finite formulation. Such a direct discrete formulation conducts to an alternative numerical method: The Cell Method. This is particularly well suited to use all the hydrogeological information available and to solve problems with complicated geome-

¹ Corresponding author: E-mail: <u>straface@dds.unical.it</u>, phone +39+0984+496572. Soil Conservation Department, The University of Calabria, 87040 Rende (CS), Italy

tries [Straface (1998)]. The present work even though introducing innovative aspects about the use of a direct discrete formulation of Richards' equation, it is one added to other sectors of application that in the last years have seen the CM affirmed for the solution of the fundamental laws of physics. The variety of such applications (fluid dynamics, solid mechanics, heat conduction and electromagnetism) is a confirmation of the generality of the method: for the way with which is formulated it is applicable to every physical theory. In elastodynamics, for example, the CM is used solve a variety of elasticity problems in which it leads to an explicit solution system, combining the advantages of a diagonal mass matrix and the possibility of using unstructured meshes [Cosmi (2005), (Han and Atluri (2004)]. In this work Cosmi has tested the convergence rate in reference to the problem of free harmonic vibrations in a system with one degree of freedom, showing that the CM has the same convergence rate of II order Runge Kutta method, but its accuracy is better. The CM results in 2D and 3D have been compared with those obtained with the commercial codes ANSYS and ABAQUS in the problem of the longitudinal vibration of a bar with free ends, for which the exact analytic solution is found in literature. The CM results are comparable with or better than those obtained with FEM, and they are particularly interesting from the point of view of computation time and memory requirements for very large meshes. Moreover, Han has developed a Meshless Local Petrov-Galerkin (MLPG) method for solving 3D elastodynamic problems. Numerical examples for solving the transient response of the elastic structures are included. The results demonstrate the efficiency and accuracy of the present method for solving the elasto-dynamic problems; and its superiority over the Galerkin Finite Element Method. The CM is used for modelling the pullout test too [Ferretti (2004)]. Various numerical models are not decisive in describing failure mechanism in pullout tests and none of the existing explanations offer a complete description of the progressive failure of the concrete medium. For this motivation, particular attention is given to the analysis in the Mohr-Coulomb plane. A failure criterion that describe crack initiation in tension loading is necessary for the analysis of the failure mechanism for the pullout test. In this work the failure analysis has been performed for several ratios between the counter pressure diameter and the stem length. The results showing how the CM can easily handle domains with several materials. Another very interesting application field of he CM regards the steady-state convectivediffusive solid-liquid phase change problem associated with temperature fields in direct-chill, semi-continuously cast billets and slabs from aluminium, based on formulation, which incorporates the mixture continuum physical model, nine-nodes support, second order polynomial trial functions, and Gaussian window weighting functions [Arler et al. (2005)]. Two-dimensional test case solution is shown, verified by comparison with the Finite Volume Method (FVM) results for coarse and fine grid arrangement. Atluri has developed a local symmetric weak form (LSWF) for linear potential problems and a truly meshless method, based on the LSWF and the moving least squares approximation, to solve potential problems with high accuracy. The method does not need a "Finite element mesh", either for purposes of interpolation of the solution variables, or for the integration of the "energy". All integrals can be easily evaluated over regularly shaped domains (in general, spheres in threedimensional problems) and their boundaries. The goodness of the several numerical examples presented in the work testify the simplicity and the great potentiality engineering applications of the method. According to principles inspiring the CM, has been developed a mathematical model for the three-dimensional flow simulation in a saturated-unsaturated porous medium. In particular, we want to show the application of the CM to solve the Richards' equation for unsaturated flow.

2 A discrete formulation of the Richards' Equation

The differential equation describing the flow in partiallysaturated porous medium, Richards' equation, is obtained combining the Darcy's equation together with the continuity equation [Bear (1979)]. For a vertical onedimensional flow in unsaturated medium, the Richards' equation is written:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left(K(\Psi) \left(\frac{\partial \Psi}{\partial z} + 1 \right) \right)$$

Assuming ψ as independent variable and introducing the absolute storage coefficient $S(\psi)$, to describe a variably-saturated medium, we have:

$$S(\Psi)\frac{\partial\Psi}{\partial t} = \frac{\partial}{\partial z}\left(K_sK_r(\Psi)\frac{\partial}{\partial z}(\Psi+z)\right)$$

where:

Ψ	Capillary head
t	Time
z	Coordinate vertical
$K(\psi)$	Hydraulic conductivity
Ks	Saturated hydraulic conductivity
$Kr(\psi)$	Relative hydraulic conductivity
$S(\psi)$	Absolute storage coefficient:
	$S ((\psi) = (d\theta / d\psi) + ((\theta (\psi) / (\phi))S$
θ	Soil moisture content
$d\theta/d\psi$	Specific capacity
¢	Porosity
Ss	Specific storage coefficient

In the equation the hydraulic conductivity, $K(\psi)$, is the product between the saturated hydraulic, Ks, and relative permeability $Kr(\psi)$. The specific storage coefficient takes into account of the porous medium deformations and is an important component in the modelling of the flow in the unsaturated zone. The Richards' equation results to be not linear because of the dependence, from the variable ψ , of the specific capacity and of the relative hydraulic conductivity.

Generally, the numerical procedures for the problem solution with initial values and to the boundary consist in a combination of space-time discretizations. When, on first step, a spatial discretization is employed (i. e. finite elements), the continuous partial differential equation is transformed in a semi-discrete system of ordinary differential equations to finite nodal points number. Successively the system of differential equations is transformed in an algebraic system of equations using the time discretization schemes.

If the original partial differential equation is not linear, unless a explicit time-discretization is used or otherwise linear, also the algebraic system will not be linear and some intermediary step required before the system can be resolved. This intermediary step generally consists in the employment of iterative-type algorithms.

The simplest approach to resolve the non linear equation of Richards numerically is that to use two levels explicit discretization. This approach produces a linear system of equations that, on basis one per-time step, represents an option to least computational cost. Nevertheless, due to stability, employing the explicit methods, it is necessary to use very small per-time steps, and therefore for long simulations or for problems that require a very fine spatial resolution (as the infiltration that involves a front of discontinuous moisture), the cost becomes excessive.

If we consider a cell complex where they have smaller dimensions there where the hypothesis of uniformity is less respected, we can employed the same constitutive equations used in the differential context as an approximation.

For that mentioned above, it follows that to obtain a discrete formulation of the fundamental equation of a physical theory, it is not necessary to go down to the differential form for then to go up again to the discreet form: it is sufficient to apply elementary physic laws in small regions where field uniformity is obtained with a degree sufficient of approximation bound, moreover, to degree of approximation imposed by input data and required to solution. Referring to concepts related to CM, the discrete formulation of the equations, which regulate the flow in porous medium, is given. For a much more complete exposition, also this formulation will be given to equations which regulate water flow in saturated zone of porous medium. In tables 1 and 2 are listed principal variables, and relative notations, used in discrete formulation.

2.1 Mass balance equation

We find the hydraulic head at all nodes at which it is not assigned: these can be internal as well as boundary vertexes. If we impose the mass balance on any dual cell, the tributary region of every vertex, we obtain as many equations as are the unknowns hydraulic heads [Paniconi et al. (1991)].

We may write the mass fluid balance as [Straface (1998)]:

$$\sum_{c \in \mathfrak{I}(h)} J_h^c + \frac{\Delta_t m_h}{\overline{\tau_h} \rho_h} = Q_h \tag{1}$$

where J_h^c is the mass flow rate, $\Delta_t m_h$ is the temporal variation of the mass content in the dual cell \overline{v}_h , ρ_h is the density of the fluid, τ_n is an interval of time and Q_h is a sink or source of mass (see Table 1). This equation simply states that in a fixed closed volume, the variation per unit time of the fluid mass is equal to the algebraic sum of the mass flow crossing the face of the dual cell. Equation (1) is valid both for interior and boundary dual cells: in this fashion, one avoids the unnatural separation

THE PRIMAL COMPLEX CELLS				
Р	point	p_h	Vertex	
L	line	l_{α}	Edge	
S	surface	s _β	Face	
V	volume	v_h	Cell	
Ι	instant	t_n	Instant	
Т	interval	τ_n	Interval	
THE DUAL CO	MPLEX CELLS			
\overline{V}	volume	\overline{v}_h	cell	
L	line	\overline{l}_{α}	edge	
\overline{S}	surface	\overline{s}_{β}	face	
\overline{P}	point	\overline{p}_h	vertex	
\overline{T}	interval	$\overline{\tau}_n$	interval	
Ī	instant	\overline{t}_n	instant	

Table 1 : Notation for space and time elements [14]

Table 2 : The global variables for the groundwater flow

CONFIGURATION VARIABLES					
Global variable	Symbol	Time element	Space element	Symbol	
Hydraulic head	Н	interval	point	$\overline{T}P$	
Head potential impulse	Λ	instant	point	ĪP	
Hydraulic gradient	8	interval	line	$\overline{T}L$	
Hydraulic conductivity	K	interval	line	$\overline{T}L$	
SOURCE VARIABLES					
Global variable	Symbol	Time element	Space element	Symbol	
Mass content	т	instant	volume	IV	
Mass flow rate	J	interval	surface	$T\overline{S}$	
Mass source	Q	interval	volume	$T\overline{V}$	

of differential equations and boundary conditions, which in this form: is typical of a differential formulation.

$$j_c = -K_c g_c \tag{2}$$

2.2 Darcy's Law

The flow rate is given by the Darcy's law. Hydraulic head H[T, P] genealogically depends on primal vertex and dual time interval, but as is obtained through a temporal variation from head impulse $\Lambda[\overline{I}, P]$, also referred to primal complexes, hydraulic head becomes function of primal instant of the time $H(t_n)$. On the other hand, the mass flow rate, that genealogically depends on a dual surface and primal interval, as is obtained from the mass content $m[\overline{I}, \overline{V}]$, it becomes function of dual instant of the time $J(\overline{t_n})$ [Troisi et al., (2000)]. We write the mass current j_c

where g_c is the hydraulic gradient that is function of the hydraulic head and its derivation depends upon the kind of interpolation used. In this work we have used a quadratic interpolation to have an high order of convergence.

$$g_c = B_c H_c \tag{3}$$

So, the mass flow rate, like the hydraulic gradient, is function of the interpolation used too and, in general, we can write [Troisi et al., (2002)]:

$$J_h^c = -A_h^c K_c g_c \tag{4}$$

2.3 The temporal variation of mass content

Temporal variation of mass content is function of the kind of flow, so we have to determine this quantity for the unsaturated flow. If we assume that water is incompressible and density independent we have:

$$\Delta_t m_h = \overline{\nu_h} \rho_h \Delta_t \theta_h = \overline{\nu_h} \rho_h \Delta_h \theta_h \Delta_t h_h \tag{5}$$

Here $\theta[I,\overline{L}]$ is the soil moisture content. Now we pose the soil moisture content variation with respect to the hydraulic head equal to $\sigma[I,\overline{V}]$. The balance equation can be written as:

$$\sum_{c \in \mathfrak{I}(h)} J_h^c + \frac{\overline{\nu_h} \sigma_h \Delta_t H_h}{\overline{\tau_h}} = Q_h \tag{6}$$

The quantity $\sigma[I, \overline{V}]$ is genealogically referred to the space dual complex and the primal instant, but, as the hydraulic head, it becomes function of dual instant of time $\sigma(\overline{t_n})$. On the other hand, the hydraulic head H_h is referred to the primal complex in time, while the mass flow rate J_h^c and the specific moisture capacity σ_h are referred to the temporal dual complex. So, as we are looking for the hydraulic head, we have to refer every quantities to the primal complex, switching the temporal elements from dual to primal:

$$t^{n+1/2} = \frac{1}{2} \left(\overline{t}^{n+1} + \overline{t}^n \right) \tag{7}$$

we obtain the mass balance equation, with the same significance of the above equation, in a discrete form:

$$\sum_{c\in\mathfrak{S}(h)} (J_h^c)^{n+1/2} + \frac{\overline{\nu_h}}{\overline{\tau_h}} \sigma_h^{n+1/2} \left(H_h^{n+1} - H_h^n \right) = Q_h \tag{8}$$

2.4 Solution of the nonlinearities

In this paper, for solving the nonlinear governing flow in variably saturated porous media, the Newton scheme, also known as Newton-Rapson iterations, is used. The Newton scheme was found to be more robust and less sensitive to nonlinearities and initial solution estimates than the Picard method. A more detailed discussion of the Newton and Picard schemes applied to the unsaturated flow equation can be found in the work by Paniconi et al. (1991).

Time step sizes during a transient simulation are dynamically adjusted according to the convergence behaviour of the nonlinear iteration scheme. A convergence tolerance, (*tol*), is specified, along with a maximum number of iteration, (*maxit*), permitted during any time step. The simulation begins with a time step of Δt_0 and proceeds until time Δt_0 . The current time step size is increased by a factor of Δt_0 (to a maximum size of Δt_{max}) if convergence is obtained in fewer than *maxit1* iterations. It is left unchanged if the convergence required between *maxit1* and *maxit2* iterations, and it is decreased by a factor of Δt_0 (to a minimum of Δt_0) if convergence required more than *maxit2* iterations.

If convergence is not obtained (*maxit* exceeded), the solution at the current time level is recomputed using a reduced time step size (factor Δt_0 , to a minimum of Δt_0). For the first time of transient simulation, or for a steady state problems, the initial conditions are used as the first solution estimate for the iterative procedure. For subsequent time step of a transient simulation the pressure head solution from the previous step is used as first estimate. The convergence is achivied when $||\Psi^{k+1,m+1} - \Psi^{k+1,m}|| \leq tol$ is satisfied.

3 Verification exercise



Figure 1 : Geometrical setting of variably saturated Test Case 1

Test Case 1. We have simulated the problem of infiltration and redistribution into a soil column initially at hydrostatic equilibrium. The boundary condition at the

r



Figure 2 : Pressure Head for Test Case 1. CM (solid line) and FEM (dashed line)

Quantity	value	Dimension
K_s	5.0	[m/s]
Θ_s	0.45	[-]
Θ_r	0.08	[-]
Ψ_s	-3.0	[m]
ψ_0	-0.19105548	[m]
n	3.0	[-]
m	0.667	[-]
S_s	0.001	$[m^{-1}]$
BDC Top	q = t/64	[m/hr]
BDC Bottom	$\psi = 0$	[m]
Δz	0.1	[<i>m</i>]
Δt	$0.005 \le \Delta t \le 1.0$	[hr]
$T_{\rm max}$	32	[hr]
$\Psi(z,0)$	-Z	[m]
Number of Nodes	1383	[-]
Number of Elements	588	
Tolerance	1×10^{-6}	[m]

Cable 3 : Values of	parameters of	the variably	saturated	Test Case 1
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surface node is a time-varying specified Darcy velocity the base node is maintained at a fixed capillary pressure q which increases linearly with time (q = t/64), while value of $\psi = 0$, allowing drainage of moisture through

Quantity	Value	Dimension
K _s	0.00922	[cm/s]
Θ_s	0.368	[-]
θ_r	0.102	[-]
n	2.0	[-]
m	0.5	[-]
α	0.0335	[-]
BDC Top	$\psi = -75$	[<i>cm</i>]
BDC Bottom	$\psi = -1000$	[<i>cm</i>]
Δz	0.25	[<i>cm</i>]
Δt	$0.1 \le \Delta t \le 3600$	[<i>s</i>]
$T_{\rm max}$	6	[hr]
$\Psi(z,0)$	-1000	[<i>cm</i>]
Number of Nodes	928	[-]
Number of Elements	1605	[-]
Tolerance	$1 x 10^{-5}$	[<i>cm</i>]

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the water table. The material properties are:

$$\theta(\psi) = \theta_r + (\theta_s - \theta_r) [1 + \beta]^{-m} \quad \psi < \psi_0$$

$$\theta(\psi) = \theta_r + (\theta_s - \theta_r) [1 + \beta_0]^{-m} + S_s (\psi - \psi_0) \quad \psi \ge \psi_0$$

$$K_r(\psi) = (1 + \beta)^{-5m/2} [(1 + \beta)^m - \beta^m]^2 \quad \psi < 0$$

$$K_r(\psi) = 1\psi \ge 0$$

with $\beta = (\psi/\psi_s)^n$ and S_s is the specific storativity coefficient. The unsaturated hydraulic conductivity versus capillary head relations were derived by van Genuchten and Nielsen (1985). The moisture content versus pressure head relations are modified versions of van Genuchten and Nielsen's expressions. The column is discretized in 588 cells (triangle) and 1383 vertexes. Mesh information and other simulation parameters are summarized in Table 3. Simulated pressure head profiles are plotted, for CM and FEM, in Fig. 2.

Test Case 2. In this case we have simulated the infiltration of water in a column. It is 30 cm high and its water content is close to that of the residual. The boundary conditions at the bottom and at the top are head fixed type. The domain of the column was subdivided with a uniform mesh (edge = 0.25 cm), so the column was discretized in 1605 cells (triangle) and 928 nodes. Mesh



Figure 3 : Geometrical setting of variably saturated Test Case 2

information and other simulation parameters are summarized in Table 4. The pressure head tolerance of Newton iterations was specified as 1×10^{-5} cm. The constitutive relations for the water content and permeability are:

$$\theta(\mathbf{\psi}) = \frac{\theta_s - \theta_r}{\left[1 + (\alpha |\psi|)^n\right]^m} + \theta_r$$

$$K_r(\mathbf{\psi}) = K_s \frac{\left\{1 - (\alpha |\psi|)^{n-1} \left[1 + (\alpha |\psi|)^n\right]^{-m}\right\}^2}{\left[1 + (\alpha |\psi|)^n\right]^{m/2}}$$



Figure 4 : Pressure Head for Test Case 2. CM (solid line) and Analytical Solution (dashed line)

Table 5 : Values of parameters of the variably saturated Test Case 3				
Quantity	Value	Dimension		
Ks	10	[cm/day]		
φ	0.45	[-]		
S _{wr}	0.333	[-]		
Ψ_a	0	[-]		
I/E	5.0	[cm/day]		
BDC Top		[m]		
BDC Bottom	$\Psi = 0$	[<i>cm</i>]		
$\Delta z = \Delta x = \Delta y$	5	[m]		
Δt	0.1	[day]		
T_{\max}	20	[day]		
$\Psi(x, y, z=0, 0)$	0	[<i>cm</i>]		
$\Psi(x, y, z = 200, 0)$	-90	[<i>cm</i>]		
$\Psi(x, y, z, 0)$	-97	[<i>cm</i>]		
Number of Nodes	3138	[-]		
Number of Elements	14293	[-]		
Tolerance	0.1	[<i>cm</i>]		

able 5 :	Values of	parameters	of the	variably	saturated	Test	Case	3
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For this test case, in literature is available the analytical solution [Philips (1969)]. Simulated pressure head profiles are plotted, for CM and Analytical solution, in Fig.

4.

Test Case 3. The problem concerns the vertical flow in the unsaturated zone above the water table. The flow re-



Figure 5 : Geometrical setting of variably saturated Test Case 3



Figure 6 : Solution for Test Case 3 (Infiltration). CM (solid line) and FEM (dashed line)

gion is represented by a rectangular soil column of dimension (50 x 50 x 200 cm) with the bottom and top faces corresponding to the water table and the soil surface, respectively (see fig. 5). The initial pressure head was assumed to be zero at the water table, -90 cm at the soil surface, and -97 cm elsewhere. The soil column was first subjected to infiltration for 10 days and then subjected to evaporation for another 10 days. The potential



Figure 7 : Solution for Test Case 3 (Evaporation). CM (solid line) and FEM (dashed line)

rates of infiltration and evaporation were assumed to be 5 cm/day [Huyakorn et al. (1986)].

We represented the flow region using a three-dimensional mesh comprising 14293 tetrahedra elements and 3138 nodes. The nodal spacing in the x, y and z directions was $\Delta x = \Delta y = \Delta z = 5cm$. The transient simulation was performed in two parts. In the first part, infiltration occurred for a period of 10 days and, in the second part the evaporation was imposed for the remaining period of 10 days. The pressure head tolerance of Newton iterations was specified as 0.1 cm.

The values of physical and geometric parameters are given in Table 5. The constitutive relations used are:

$$K_r(\Psi) = (S_w - S_{wr}) / (1 - S_{wr})$$

$$(\psi - \psi_a)/(-100 - \psi_a) = (1 - S_w)/(1 - S_{wr})$$

Simulated pressure head profiles during infiltration and subsequent evaporation are plotted, for CM and FEM, in Fig. 6 and 7 respectively.

4 Conclusions

In this work we present an alternative to the classical differential type approach to the solution of Richards'

Equations. This alternative is based on a preliminary reformulation of the mathematical model in a partially discrete form which preserves as much as possible the physical and geometrical content of the original problem. It is made possible by the existence and properties of a common mathematical structure of physical field theories [Tonti (1975)]. The goal is to maintain the focus, both in the modelling and in the discretization step, on the physics of the problem, thinking in terms of numerical methods for physical field problems, and not of a particular mathematical form into which the original problems happens to be translated [Mattiussi (1997)]. It is customary to derive a finite formulation of the groundwater flow equation passing through differential formulation. The paper has shown that is possible to obtain a finite formulation starting directly from experimental laws. This is accomplished using global variables and realizing their natural association with space and time elements. In such an association important role is played by the notions of inner and outer orientations of a space and time element. This leads us to use a cell complex and its dual instead of a coordinate system. Once the variable of groundwater hydraulics are classified in one of the three classes, configuration, source and energy variables, it is seen that configuration variables are naturally referred to the cells of a primal complex while source variables are referred to those of the dual complex. Constitutive equations, that link configuration with source variables, require the introduction of mean densities and mean rates. The approximation of considering the field inside every cell of the primal complex as uniform permits us to avoid the limit process. The procedure presented here is not peculiar to groundwater hydraulics but also in fluid dynamics, in solid mechanics, in heat conduction and in electromagnetism, as shown in references [Tonti (2001)]. The scheme here presented gives a second order accuracy on a structure mesh. It has been proved that using parabolic interpolation functions inside every triangle one can obtain a fourth order accuracy on structured meshes.

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