Chapter 7

Hydromechanical coupling theory in unsaturated geomaterials and its numerical integration

7.1. Introduction – problems to be treated

We are here interested in a number of different physical phenomena, including:

- the non-linear solid mechanics, and especially the soil, rock or concrete mechanics: we consider the relations between displacements, strains, stresses and forces within solids. The material behaviour is described by a constitutive model, which can take into account elastoplasticity or elasto-visco-plasticity. On the other hand, large transformations and large strains may lead to geometrical non-linearities.
- the fluid flow within porous media: fluid can be a single phase of various natures (water, air, gas, oil …) or it can be an association of two fluids, leading to unsaturated media (water and air, oil and gas, oil and water…). In the second case, partial saturation is leading to permeability and storage terms depending on the saturation degree or on the suction level, involving non-linear aspects.
- the thermal transfers within porous media. Conduction is the leading process in solid (in the geomaterial matrix), but convection can also occur in the porous volume, as a consequence of the fluid flow. Radiation transfer could also

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occur inside the pores, but it will be neglected here. Conduction coefficients and latent heat may depend on the temperature.

- the pollutant transport or any spatial transfer of substance (including heat, dissolved gas, etc.) thanks to the fluid flow. The pollutant concentration may be high enough to modify the densities, involving non-linear effects.

All these problems are non-linear ones, and can be formulated with sets of partial differential equations. Moreover only three types of differential equations have to be considered, concerning respectively i) solid mechanics, ii) diffusion and iii) advection-diffusion problems.

7.1.1. Solid mechanics

On the one hand, solid mechanics can be modelled on the following basis. The equilibrium equation is:

$$\partial_i \sigma_{ij} + P_j = 0 \qquad [1]$$

where $\underline{P}$ is the vector of volume forces, $\underline{\underline{\sigma}}$ is the Cauchy's stress tensor and $\underline{\partial}$ represents the spatial partial derivative operator:

$$\partial_i \equiv \frac{\partial}{\partial x_i} \qquad [2]$$

The stress tensor is obtained thanks to the time integration of a (elastic, elastoplastic, damage or elasto-visco-plastic) constitutive equation, possibly including coupling terms [COU 95, COU 04, ALO 90, COL 05, BER 08]:

$$\overset{\circ}{\sigma}_{ij} = fct(\sigma, D, k) \qquad [3]$$

where $\underline{\overset{\circ}{\sigma}}$ is the stress rate, $\underline{D}$ is the strain rate and k is a set of history parameters (state variables, as eg. the preconsolidation stress). In the most classical case of elastoplasticity, this equation reduces to:

$$\overset{\circ}{\sigma}_{ij} = C_{ijkl} D_{kl} \qquad [4]$$

Most constitutive equations for geomaterials are non-linear ones.

When modelling a solid mechanics problem with the finite element method, the most used formulation is based on displacements $\underline{u}$ or on actualised coordinates $\underline{x}$. If one considers only small strains and small displacements, the strain rate reduces to the well-known Cauchy's strain rate:

$$D_{ij} = \dot{\varepsilon}_{ij} = \frac{1}{2}\left(\partial_i \dot{u}_j + \partial_j \dot{u}_i\right) \quad [5]$$

However, if large strains are to be considered, the preceding equations have to be reconsidered. The stress – strain rate couple has to be more precisely defined, with respect to the configuration evolution. Among multiple other choices (cf. Piola-Kirchoff stress – Green strain), we will only consider here the Cauchy's stress and the Cauchy's strain rate. These tensors are defined in global axis in the current configuration, which is continuously deforming. If we note $\underline{X}$ the coordinates in a reference state (an initial one; however initial state in geomechanics is always arbitrary), and $\underline{x}$ the coordinates in the current configuration (Figure 7.1), we can define the Jacobian tensor of the transformation:

$$F_{ij} = \frac{\partial x_i}{\partial X_j} \quad [6]$$

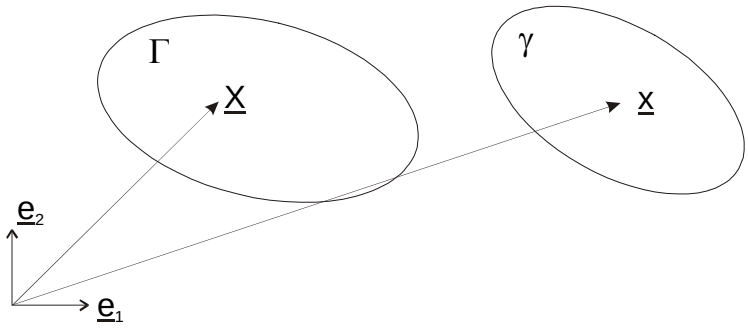

Figure 1. *Initial and current configurations*

The velocity gradient is defined as:

$$\underline{L} = \frac{\partial \underline{u}}{\partial \underline{X}} = \dot{\underline{F}} \ \underline{F}^{-1} \quad [7]$$

The symmetric part of the velocity gradient is the strain rate associated to the Cauchy's stress :

$$\underline{D} = sym(\underline{L}) = \frac{1}{2}\left(\underline{L} + \underline{L}^T\right) \quad [8]$$

The material stress evolution must then be described as a function of the strain rate, thanks to a constitutive equation [3]. However, as the Cauchy's stress tensor is defined in global axis, the solid rotations will modify the tensor Cartesian components. This evolution is not linked to strains and so is not described by the constitutive equation. Among other possibilities, the Jaumann's objective derivative of the stress is a good component update:

$$\dot{\underline{\sigma}} = \frac{D\underline{\sigma}}{dt} = \breve{\underline{\sigma}} + \underline{\omega}\ \ \underline{\sigma} + \underline{\sigma}\ \ \underline{\omega}^T \quad [9]$$

$$\underline{\omega} = skw(\underline{L}) = \frac{1}{2}\left(\underline{L} - \underline{L}^T\right) \quad [10]$$

Such large strain model [6-10] is non-linear.

Time dimension is not to be addressed for solid mechanics problems, unless when viscous term are considered in the constitutive model. Generally, the time that appears in the time derivatives in [3,4,5,7-10] is only a formal one.

7.1.2. Diffusion

Fluid flow in porous media and thermal conduction exchanges in solids are modelled thanks to similar diffusion equations.

The balance equation writes:

$$\partial_i f_i + Q = \dot{S} \quad [11]$$

where $\underline{f}$ represents a flux of fluid or of heat, Q represents a sink term and S represents the storage of fluid or of heat. When modelling a diffusion problem with the finite element method, the most used formulation is based on fluid pore pressure p or on temperature T.

Then the Darcy's law for fluid flow in porous media gives the fluid flux:

$$f_i = -\frac{k}{\mu}(\partial_i p + \partial_i \rho g z) \quad [12]$$

with the intrinsic permeability k (possibly depending on the saturation degree), the dynamic viscosity μ, the density ρ, and the gravity acceleration g. The fluid storage term depends on the saturation degree S_r and on the fluid pressure:

$$\dot{S} = fct(p, S_r) \quad [13]$$

For thermal conduction one obtains the Fourier's law:

$$f_i = -\lambda \ \partial_i T \quad [14]$$

with the conductivity coefficient λ. The heat storage (enthalpy) term depends on the temperature:

$$\dot{S} = fct(T) \quad [15]$$

The diffusion problem is non linear when:

- the permeability depends (directly or indirectly) on the fluid pore pressure;
- the fluid storage is a non-linear function of the pore pressure;
- partial saturation occurs;
- the conductivity coefficient depends on the temperature;
- the enthalpy is a non-linear function of the temperature.

When the storage term is considered, time dimension of the problem has to be addressed.

7.1.3. Advection – diffusion

Transport of pollutant or of heat in porous media is governed by a combination of advection and diffusion [COL 03, CHA 01, COL 02, GEN 01a, LI 97, LEW 00]. Advection phenomenon is related to the transport (noted as a flow f_{adv}) of any substance by a fluid flow, described by its velocity $\underline{f}_{diff}^{fluid}$:

$$\underline{f}_{adv} = C \ \ \underline{f}_{diff}^{fluid} \qquad [16]$$

The substance concentration C is generally supposed to be small enough not to influence the fluid flow. In porous media, due to the pores network tortuosity and to the friction, advection is always associated to a diffusion characterised by diffusion – dispersion tensor $\underline{D}$. Therefore, the total flux of substance is:

$$f_{i,adv-diff} = C\, f_{i,diff}^{fluid} - \lambda D_{ij} \partial_j C \qquad [17]$$

Balance equation and storage equations may be written in a similar way to the one for diffusion problems [11,13,15].

Compared to diffusion constitutive law [12,14], it appears here an advection term which doesn't depend on the concentration gradient, but directly on the concentration. This is modifying completely the nature of the equations to be solved. Problems dominated by advection are very difficult to solve numerically [CHA 01]. In order to evaluate the relative advection effect, it is useful to evaluate the Peclet's number, which is a ratio between diffusive and advective effects:

$$Pe = \frac{f_{diff}^{fluid} h}{2D} \qquad [18]$$

where h is an element dimension.

7.1.4. Boundary conditions

In the preceding section, differential equations are given for three types of problems. Solving these equations needs to define boundary and initial conditions. Classical boundary conditions may be considered : imposed displacements or forces for solid mechanics problems, imposed fluid pressures / temperatures / concentrations or imposed fluxes for diffusion and advection – diffusion problems.

However, it may be useful to consider much complex boundary conditions. For example, in solid mechanics, unilateral contact with friction or interface behaviour is often to be considered [CHA 90].

On the other hand, initial conditions are often difficult to determine in geomechanics, as for example the problem of initial stress state.

7.2. Numerical tools : the finite element method

7.2.1. Introduction

An approximated solution of most problems described by a set of partial differential equations may be obtained thanks to numerical method like the finite element method (FEM), the discrete element method (DEM), the finite difference method (FDM), the finite volume method (FVM) or the boundary element method (BEM). For the problems concerned here, the most used methods are the finite element one and the finite difference one.

Non-linear solid mechanics is better solved thanks to the finite element method. Boundary element methods have strong limitation in the non-linear field. Finite difference methods are not easy to apply to tensorial equations (with the exception of the FLAC code, developed by Itasca).

Diffusion and advection – diffusion problems are often solved by finite difference or finite element method. Some finite difference codes are very popular for fluid flow, as eg. *MODFLOW* for aquifer modelling or *ECLIPSE* [ECL 00] for oil reservoir modelling. These codes have been developed for a number of years and posses a number of specific features allowing taking numerous effects into account. However, they suffer from some drawbacks, which limit their potentialities for modelling coupled phenomena. Therefore we will only give little information about finite differences.

7.2.2. Finite element method

The basic idea of the finite element method is to divide the field to be analysed into sub-domains, the so-called *finite elements*, of simple shape: eg. triangles, quadrilaterals with linear, parabolic, cubic sides for two-dimensional analysis. In each finite element, an analytical simple equation is postulated for the variable to be determined, i.e. the coordinate or displacement for solid mechanics, and the fluid pressure, temperature, concentration for diffusion problems. In order to obtain C_0 continuity, the unknown variable field has to be continuous at the limit between finite elements. This requirement is obtained thanks to common values of the field at specific points, the so-called *nodes*, which are *linking* the finite elements together. The field values at nodal points are the discretised problem unknowns.

For most solid mechanics and diffusion problems, isoparametric finite elements seem to be optimal [ZIE 89]. The unknown field $\underline{x}$ may then be written, for solid mechanics cases in two-dimensional cases:

$$\underline{x} = N_L(\xi,\eta)\ \ \underline{x}_L \quad L = 1, nnode \qquad [19]$$

It depends on the nodal unknowns $\underline{x}_L$ and on shape functions N_L, themselves depending on isoparametric coordinates ξ, η defined on a reference normalised space. Then the strain rate and the spin may be derived thanks to equations [8] and [10], the stress rate is obtained by [3], [4] and [9] and is time integrated. Eventually, equilibrium [1] has to be checked (section 7.2.4).

For scalar diffusion or advection – diffusion problems, the unknown field p (we will use hereafter the pore pressure notation, however temperature T or concentration C could be also considered changing the notation) may then be written:

$$p = N_L(\xi,\eta)\ \ p_L \quad L = 1, nnode \qquad [20]$$

It depends on the nodal unknowns p_L and on shape functions N_L. Then the fluid Darcy's velocity and the storage evolution may be derived thanks to equations [12] and [13] (respectively [14-15] or [16-17]). No time integration is required here. Eventually, balance equation [11] has to be checked (section 7.2.4).

The finite element method allows an accurate modelling of the boundary condition, thanks to easily adapted finite element shape. Internal boundaries of any shape between different geological layers or different solids can be modelled. Specific finite elements for interfaces behaviour or for unilateral boundaries may have also been developed [CHA 90]. Variations of the finite element size and density over the mesh are also easy to manage thanks to present mesh generators.

7.2.3. Finite difference method

The finite difference method doesn't postulate explicitly any specific shape of the unknown field. As we are concerned with partial differential equations, exact derivative are replaced by an approximation based on neighbour values of the unknown:

$$\left(\frac{\partial p}{\partial x}\right)_i = \frac{p_{i+1} - p_{i-1}}{2h} \qquad [21]$$

where the subscript $_i$ denotes the cell number and h denotes the cell size. For an orthogonal mesh, such derivatives are easily generalised to variable cell dimensions. However non-orthogonal meshes are asking question highly difficult to solve and

are generally not used. Boundary conditions have then to be modelled by the juxtaposition of orthogonal cells, giving a kind of stairs for oblique or curved boundaries. Similarly, local refinement of the mesh induces irreducible global refinement. These aspects are the most prominent drawbacks of the finite difference method compared to the finite element one. On the other hand, computing time is generally much lower with finite differences then with finite elements.

7.2.4. Solving the non- linear problem: the Newton-Raphson method

Let us now concentrate on the finite element method. The fundamental equation to be solved is the equilibrium equation [1] (respectively the balance equation [11] for diffusion phenomena). As the numerical methods are giving an approximated solution, the equilibrium / balance equation has to be solved with the best compromise. This is obtained thanks to a global weak form of the local equation. Using weighted residuals, one obtains for solid mechanics:

$$\int_V \left[\sigma_{ij} \ \delta\varepsilon_{ij} \right] dV = \int_V P_i \ \delta u_i \ dV + \int_A \overline{p} \ \delta u_i \ dA \qquad [22]$$

and for diffusion phenomena:

$$\int_V \left[\dot{S} \ \delta p - f_i \ \partial_i (\delta p) \right] dV = \int_V Q \ \delta p \ dV + \int_A q \ \delta p \ dA \qquad [23]$$

where $\overline{p}$ and q are surface terms of imposed loads / fluxes. The weighting functions are denoted $\underline{\delta u}$ and δp, and $\underline{\delta\varepsilon}$ represents a derivative of the weighting function based on the Cauchy's strain derivate operator. An equivalent equation could be obtained based on the virtual power principle. The $\underline{\delta u}$ and δp would then be interpreted as virtual arbitrary displacements and pressures. Within the finite element method, these global equilibrium / balance equation will be verified for a number of fundamental cases equivalent to the degrees of freedom (dof) of the problem, i.e. the number of nodes times the number of freedom degrees per node, minus to imposed values. The corresponding weighting functions will have simple forms based on the element shape functions (for Galerkin's approximation; for advection dominated problems, other weighting functions have to be used).

Giving a field of stress or of flux, using the weighting functions, one will obtain a value for each dof, which is equivalent to a nodal expression of the equilibrium / balance equation. More precisely, for solid mechanics problems, one will obtain internal forces equivalent to stresses:

$$F_{Li}^{\text{int}} = \int_V \sigma_{ij} B_{Lj} dV \qquad [24]$$

where B is a matrix of derivatives of the shape functions N. If equilibrium is respected from the discretised point of view, these internal forces are equal to external forces (if external forces are distributed, a weighting is necessary):

$$F_{Li}^{\text{int}} = F_{Li}^{ext} \qquad [25]$$

Similarly, for diffusion phenomena, the nodal internal fluxes are equivalent to the local fluxes:

$$F_L^{\text{int}} = \int_V \left[\dot{S} N_L - f_i \partial_i N_L \right] \, dV \qquad [26]$$

If the balance equation is respected from the discretised point of view, these internal fluxes are equal to external ones:

$$F_{Li}^{\text{int}} = F_{Li}^{ext} \qquad [27]$$

However, as we are considering non linear-problems, equilibrium / balance cannot be obtained immediately, but needs to iterate. This means that the equations [25,27] are not fulfilled until the last iteration of each step.

Non-linear problems are solved for some decades, and different methods have been used. From our point of view, the Newton – Raphson is the reference method and probably the best one for a large number of problems. Let us describe the method. In the equation [25], the internal forces F_L^{int} are depending on the basic unknown of the problem, i.e. the displacement field. Similarly in equation [27] the internal fluxes are depending on the pressure (temperature, concentration…) field.

If they don't equilibrate the external forces / fluxes, the question to be treated can be formulated under the following form:

How should we modify the displacement field (the pressure field) in order to improve the equilibrium (the balance) as stated by equation [25,27] ?

Following the Newton – Raphson method, one develops the internal force as a first order Taylor's series around the last approximation of the displacement field:

$$F_{Li}^{\text{int}} = F_{Li}^{\text{int}}(u_{(i)}) + \frac{\partial F_{Li}^{\text{int}}}{\partial u_{Kj}} du_{Kj} + O^2 = F_{Li}^{ext} \qquad [28]$$

This is a linearisation of the non-linear equilibrium equation. It allows obtaining a correction of the displacement field:

$$\Delta u_{Kj} = \left(\frac{\partial F_{Li}^{\text{int}}}{\partial u_{Kj}} \right)^{-1} \left(F_{Li}^{\text{int}}(u_{(i)}) - F_{Li}^{ext} \right) = K_{Li,Kj} \left(F_{Li}^{\text{int}}(u_{(i)}) - F_{Li}^{ext} \right) \qquad [29]$$

The matrix noted $K_{Li,Kj}$ is the so-called stiffness matrix. With the corrected displacement field, one may evaluate new strain rates, new stress rates and new improved internal forces. Equilibrium should then be improved.

The same meaning may be developed for diffusion problems: Taylor's development of the internal fluxes with respect to the pressures / temperatures / concentrations nodal unknowns.

The iterative process may be summarised as shown on Figure 7.2 for one-dof solid mechanics problem. Starting from a first approximation of the displacement field $u_{(1)}$, one computes the internal forces $F_{L(1)}^{\text{int}}$ (point $A^{(1)}$) that are lower then the imposed external forces F_L^{ext}. Equilibrium is then not fulfilled and a new approximation of the displacement field is searched. The tangent stiffness matrix is evaluated and an improved displacement is obtained $u_{(2)}$ (point $B^{(1)}$) [29]. One computes again the internal forces $F_{L(2)}^{\text{int}}$ (point $A^{(2)}$) that are again lower then the external forces F_L^{ext}. As equilibrium is not yet fulfilled, a new approximation of the displacement field is searched $u_{(3)}$ (point $B^{(2)}$). The procedure has to be repeated until the equilibrium / balance equation is fulfilled with a given accuracy (numerical convergence norm). The process has a quadratic convergence, which is generally considered as the optimum numerical solution.

However the Newton–Raphson method has an important drawback : it needs important work to be developed as well as to be run on a computer. Especially the stiffness matrix K is time consuming for the analytical development and for the numerical inversion. Therefore other methods have been proposed:

- approximate stiffness matrix, in which some non-linear terms are neglected;
- successive use of the same stiffness matrix avoiding new computation and inversion at each iteration.

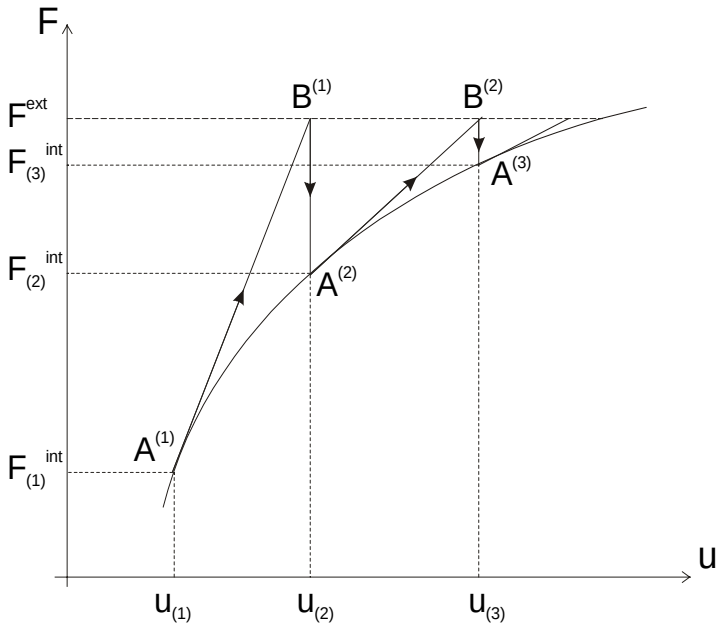

Figure 2. *Illustration of the Newton–Raphson process*

It should be noted that each alternative is reducing the numerical convergence rate. For some highly non-linear problems, the convergence may be loosed, and then no numerical solution may be obtained.

Some other authors, considering the properties and the efficiency of explicit time schemes in rapid dynamic (like for shocks modelling) add an artificial mass to the problem in order to solve it as a quick dynamic one. It should be clear that such technique might degrade the accuracy of the solution, as artificial inertial effects are added and the static equilibrium equation [1] is not checked.

7.2.5. The stiffness matrix

From equation [29], it appears that the stiffness matrix is a derivative of the internal forces:

$$K_{Li,Kj} = \frac{\partial F_{Li}^{\text{int}}}{\partial u_{Kj}} = \frac{\partial}{\partial u_{Kj}} \left(\int_V \sigma_{ij} B_{Lj} dV \right) \quad [30]$$

Two contributions will be obtained. On the one hand, one has to derive the stress state with respect with the strain field, itself depending on the displacement field. On the other hand, the integral is performed on the volume and the *B* matrix depends on the geometry. If we are concerned with large strains and if we are using the Cauchy's stresses, geometry is defined in the current configuration, which is changing from step to step, and even from one iteration to the other. These two contributions, the material one, issued from the constitutive model, and the geometric one have to be accurately computed in order to guaranty the quadratic convergence rate.

A similar discussion may be given for diffusive problems. However, the geometry is not modified for pure diffuse problems, so only the material term is to be considered.

7.2.6. Transient effects: the time dimension

Time dimension appears in first order time derivative in the constitutive mechanical model [3,9] and in the diffusion problems through the storage term. We will here discuss the time integration procedure and the accuracy and stability problems that are involved.

7.2.6.1. Time integration – diffusion problems

The period to be considered is divided in time steps. Linear evolution of the basic variable with respect to the time is generally considered within a time step:

$$p = \frac{t - t_A}{t_B - t_A} p_B + \frac{t_B - t}{t_B - t_A} p_A \quad [31]$$

where the subscripts $_{A,B}$ denote respectively the beginning and the end of a time step. Then the pressure rate is:

$$\dot{p} = \frac{dp}{dt} = \frac{p_B - p_A}{t_B - t_A} = \frac{\Delta p}{\Delta t} \quad [32]$$

This time discretisation is equivalent to a finite difference scheme. It allows evaluating any variable at any time within a time step.

The balance equation should ideally be fulfilled at any time during any time step. Of course this is not possible for a discretised problem. Only a mean assessment of the balance equation can be obtained. Weighted residual formulations have been proposed in a similar way as for finite elements [ZIE 89]. However the implementation complexity is too high with respect to the accuracy. Then the easiest solution is to assess only the balance equation at a given time noted θ inside the time step:

$$\theta = \frac{t_\theta - t_A}{t_B - t_A} \qquad [33]$$

All variables have then to be evaluated at the reference time θ. Different classical schemes have been discussed for some decades:

- fully explicit scheme - $\theta = 0$: all variables and the balance are expressed at the time step beginning, where everything is known (solution of the preceding time step). The solution is therefore apparently very easy to be obtained;
- Crank-Nicholson scheme or mid-point scheme - $\theta = 1/2$;
- Galerkin's scheme - $\theta = 2/3$;
- fully implicit scheme - $\theta = 1$.

The last three schemes are function of the pore pressure / temperature / concentration at the end of the time step, and may need to iterate if non-linear problems are considered.

For some problems where rapid change of material properties occurs, difficulties in the modelling could appear. For instance, problems where phase changes occur as icing or vaporising of water) are associated to latent heat consummation and abrupt change of specific heat and thermal conductivity. Such rapid change is not easy to model. The change in specific heat may be smoothed using an enthalpy formulation, because enthalpy H is an integral of the specific heat c. Then finite difference of the enthalpy evaluated over the whole time step gives a mean value $\overline{c}$ and so allows accurate balance equation:

$$H = \int_T c \; dT \qquad [34]$$

$$\overline{c} = \frac{H_B - H_A}{t_B - t_A} \qquad [35]$$

7.2.6.2. Time integration – solid mechanics

For solid mechanics problems, the constitutive law form [3,4] is an incremental one at the difference with the ones for diffusion problems [12]. The knowledge of the stress tensor at any time implies to have time integrated the constitutive law. The stress tensor is a state variable that is stored and transmitted from step to step based on its final / initial value, and this value plays a key role in the numerical algorithm.

Then, in quite all finite element code devoted to modelling, equilibrium is expressed at the end of the time steps, following then a fully implicit scheme - $\theta = 1$, and using the end of step stress tensor value.

However, integrating the stress history with enough accuracy is crucial for the numerical process stability and global accuracy. Integrating the first order differential equation:

$$\underline{\sigma}^{B} = \underline{\sigma}^{A} + \int_{t^A}^{t^B} \underline{\underline{C}}^{ep} \, \underline{\dot{\varepsilon}} \; dt \qquad [36]$$

can be based on similar concepts as the one described in the preceding paragraph. Various time schemes based on different θ values may be used. Stability and accuracy discussion (section 7.2.6.3) are similar.

When performing large time steps, obtaining enough accuracy may require to use sub-stepping: within each global time step (as regulated by the global numerical convergence and accuracy problem), the stress integration is performed at each finite element integration point after division of the step in a number a sub-steps allowing high accuracy and stability.

7.2.6.3. Scheme accuracy

The theoretical analysis of a time integration scheme accuracy and stability is generally based on a simplified problem [ZIE 89]. Let consider diffusion phenomena restricted to linear case. Introducing the discretised field [20] into the constitutive equations gives for the Darcy law (neglecting here the gravity term for the sake of simplicity):

$$f_i = -\frac{k}{\mu} \partial_i p = -\frac{k}{\mu} (\partial_i N_L) \, p_L \qquad [37]$$

Similarly the storage law (linear case) gives:

$$\dot{S} = c \;\; \dot{p} = c \;\; N_L \;\; \dot{p}_L \tag{38}$$

where c is a storage parameter. Neglecting source terms, the weak form of the balance equation [23] writes then

$$\begin{aligned} &\int_V \left[\dot{S} \;\delta p - f_i \;\partial_i (\delta p) \right] dV \\ &= \int_V c \; N_L \; \dot{p}_L \; N_K \; \delta p_K \; dV - \int_V - \frac{k}{\mu} \partial_i N_L \; p_L \; \partial_i N_K \; \delta p_K \; dV = 0 \end{aligned} \tag{39}$$

Considering that nodal values are not concerned by the integration, it comes:

$$\begin{aligned} &\left(\int_V c \; N_L \; N_K \; dV \right) \dot{p}_L \; \delta p_K + \left(\int_V \frac{k}{\mu} \partial_i N_L \; \partial_i N_K \; dV \right) p_L \; \delta p_K \\ &= C_{KL} \; \dot{p}_L \; \delta p_K + K_{KL} \; p_L \; \delta p_K = 0 \end{aligned} \tag{40}$$

which is valid for any arbitrary perturbation $\underline{\delta p}$. Then:

$$C_{KL} \dot{p}_L \;\; + K_{KL} p_L = 0 \tag{41}$$

which is a simple system of linear equations with a time derivative, a storage matrix $\underline{\underline{C}}$ and a permeability matrix $\underline{\underline{K}}$. One can extract eigenvalues of this system and so arrive to a series of scalar independent equations of similar form:

$$\dot{p}_L + \alpha_L^2 p_L = 0 \quad \text{(no summation)} \tag{42}$$

where L represents now the number of the eigenmode with the eigenvalue α_L and will not be noted in the following. The exact solution for equation [42] is a decreasing exponential:

$$p(t) = p(t_0) e^{-\alpha^2 t} \tag{43}$$

This problem represents then the damping of a perturbation for a given eignemode. Numerically, the modelling is approximated and numerical errors always appear. If the equation [43] is well modelled, any numerical error will be rapidly damped, if the error source is not maintained. Following this analysis, the

whole accuracy and stability discussion may be given on these last scalar equations [42,43].

Introducing the time discretisation [32,33] in [42] gives :

$$\frac{p_B - p_A}{\Delta t} + \alpha^2 \left[(1-\theta) p_A + \theta p_B \right] = 0 \qquad [44]$$

which allows to evaluate the end of step pressure as a function of the beginning of step one:

$$p_B = A\, p_A \qquad [45]$$

with the amplification factor:

$$A = \frac{1-(1-\theta)\alpha^2 \Delta t}{1+\theta \alpha^2 \Delta t} \qquad [46]$$

To ensure the damping process of the numerical algorithm, which is the *stability condition*, it is strictly necessary that the amplification factor remains lower then unity:

$$-1 < A < 1 \qquad [47]$$

This condition is always verified if $\theta \geq ½$, and conditionally satisfied otherwise:

$$\Delta t \leq \frac{2}{(1-2\theta)\alpha^2} \quad \text{if } \theta < ½ \qquad [48]$$

This last equation is not easy to verify, as it depends on the eingenvalues, which are generally not computed. Therefore, for classical diffusion process considered in geomaterials, the condition $\theta \geq ½$ is generally used.

It should be noted that the amplification factor becomes negative for large time steps, unless for the fully implicit scheme. Then the pertubated pressure decreases monotically in amplitude but with changes of sign. This may be questionable for some coupled phenomena, as it could induce oscillation of the coupled problem.

Let us now consider the accuracy of the numerical schemes. Developing in Taylor's series the exact and numerical solution allows to compare them:

$$A_{exact} = 1 - x + \frac{1}{2}x^2 - \frac{1}{6}x^3 + \ldots$$
$$A_{\text{numérique}} = 1 - x + \theta x^2 - \theta^2 x^3 + \ldots \qquad [49]$$
$$x = \alpha^2 \Delta t$$

It appears that the only Crank-Nicholson scheme θ = ½ has second order accuracy properties. However this conclusion is limited to infinitesimal time steps. For larger time steps, as in most numerical models, the Galerkin's scheme θ = 2/3 gives the optimal compromise and should be generally used.

The whole discussion related to the stability and accuracy of the proposed time numerical schemes was based on eigenmodes of a linear problem. Can we extrapolate them to general problems? The eigenvalue passage is only a mathematical tool to be able to consider scalar problems, and has no influence on our conclusions. Oppositely, the non-linear aspects could modify sometimes our conclusions. However, it is impossible to develop the analysis for a general non-linear problem, and the preceding conclusions should be adopted as guidelines, as they appear to be fruitful in most cases.

7.2.7. Advection diffusion processes

Let us first consider a purely advective process. Then the transport is governed by the advection equation [16] and by the balance equation [11]. Associating these two equations, on obtains:

$$(\underline{\nabla}^T C).\underline{f}_{diff}^{fluid} + \dot{C} = 0 \qquad [50]$$

which is a hyperbolic differential equation. It cannot be solved by the finite element or finite difference problem, but by characteristic methods. The idea is to follow the movement of a pollutant particle by simply integrating step by step the fluid velocity field. This integration has to be accurate enough, as errors are cumulated from one step to the next. On the other hand, if advection is very small compared to diffusion, then the finite element and finite difference methods are really efficient.

For most practical cases, an intermediate situation holds. It can be checked by the Peclet's number [18], which is high for mainly advective processes and low for mainly diffusive one. As diffusion has to be taken into account, the numerical solution must be based on the finite element method (the finite difference one may also be used but will not be discussed here). However, numerical experiments show that the classical Galerkin's formulation gives very poor results with high spatial oscillations and artificial dispersion. Then new solutions have been proposed [ZIE

89, CHA 01]. A first solution is based on the use in the weighted residual method of weighting function that differs from the shape one by an upwind term, i.e. a term depending in amplitude and direction on the fluid velocity field. The main advantage of this method is to maintain the finite element code formalism. However, it is never possible to obtain a highly accurate procedure. Numerical dispersion will always occur.

Other solutions are based on the association of the characteristic method for the advection part of the process and of the finite element method for the diffusive part [LI 97]. The characteristic method may be embedded in the finite element code, what has a strong influence on the finite element code structure. It is also possible to manage the two methods in separated codes, as in a staggered procedure (section 7.3.3.).

7.3. Coupling various problems

7.3.1. Finite element modelling: monolithical approach

Modelling the coupling between different phenomena should imply to model each of them and, simultaneously, all the interactions between them. A first approach consists in developing new finite elements and constitutive laws especially dedicated to the physical coupled problem to be modelled. This approach allows taking accurately all the coupling terms into account. However there are some drawbacks that will be discussed in a later section.

The number of basic unknowns and following the number of degrees of freedom – dof per node are increased. This has a direct effect on the computer time used for solving the equation system (up to the third power of the total dof number). Coupled problems are highly time consuming. Isoparametric finite element will often be considered. However some specific difficulties may be encountered for specific problems. Nodal forces or fluxes are computed in the same way as for decoupled problems (section 7.2.4). However stiffness matrix evaluation is much more complex, as interactions between the different phenomena are to be taken into account. Remember that the stiffness or iteration matrix [29] is the derivative of internal nodal forces / fluxes with respect to the nodal unknowns (displacements / pressures / …). The complexity is illustrated by the following scheme of the stiffness matrix, restricted to the coupling between two problems:

Derivative of problem **1** nodal forces with respect to problem **1** nodal unknowns	Derivative of problem **1** nodal forces with respect to problem **2** nodal unknowns
Derivative of problem **2** nodal forces with respect to problem **1** nodal unknowns	Derivative of problem **2** nodal forces with respect to problem **2** nodal unknowns

The part of the stiffness matrix in cells 1-1 and 2-2 are similar or simpler to the ones involved in uncoupled problems. The two other cells 1-2 and 2-1 are new and may be of certain complexity. Remember also that the derivative consider internal nodal forces / fluxes as obtained numerically, i.e. taking into account all numerical integration / derivation procedures. On the other hand, large difference of orders of magnitude between different terms may cause troubles in solving the problem and so need to be checked.

Numerical convergence of the Newton–Raphson process has to be evaluated carefully. It is generally based on some norms of the out-of-balance forces / fluxes. However, coupling implies often mixing of different kinds of dof, which may not be compared without precaution. Convergence has to be obtained for each basic problem modelled, not only for one, which would then predominate in the computed indicator.

7.3.2. Physical aspects: various terms of coupling

A large number of different phenomena may be coupled. It is impossible to discuss here all potential terms of coupling, and we will restrict ourselves to some basic cases often implied in environmental geomaterial mechanics. In the following paragraphs, some fundamental aspects of potential coupling are briefly described. More information can be obtained in dedicated chapters of this book.

7.3.2.1. Hydromechanical coupling

Coupling mechanical deformation of soils or rock mass and water flow in pores is a frequent problem in geomechanics. Three dof per node are needed for 2D analysis (2 displacements + 1 pore pressure) and four dof for 3D analysis (3 displacements + 1 pore pressure).

The first coupling terms are related to the influence of pore pressure on mechanical equilibrium through the Terzaghi's postulate:

$$\underline{\sigma} = \underline{\sigma'} + p\underline{I} \qquad [51]$$

with the effective stress tensor $\underline{\sigma'}$ related to the strain rate tensor thanks to the constitutive equation [3], and the unity tensor $\underline{I}$. For unsaturated geomaterials, the effective stress concept has to be discussed [BIS 59, COU 95, COU 04, NUT 08] and generally additional variables have to be considered [FRE 77].

The second type of coupling concerns the influence of the solid mechanics behaviour on the flow process, which comes first through the storage term. Storage of water in saturated media is mainly due to pores strains, i.e. to volumetric changes in soil / rock matrix:

$$\dot{S} = \dot{\varepsilon}_v \qquad [51]$$

A other effect, which may be considered, is the permeability change related to the pore volume change, which may for example be modelled by the Kozeni – Carman law as a function of the porosity $k = k(n)$. In EDZ – excavation damaged zone around tunnels, the presence of micro or macro fractures has a much stronger effect and may change permeability of several orders of magnitude [LEV 10, OLI 08].

Biot proposed an alternative formulation for rocks where contacts between grains are much more important then in soils. Following Biot, the coupling between flow and solid mechanics are much more important [DET 91, BIO 41].

Other numerical problems could occur with the time dimension. First implicit scheme are used for the solid mechanics equilibrium and various solutions are possible for the pore pressure diffusion process. Consistency would imply to use fully explicit schemes for the two problems. Moreover, it has been shown (section 7.2.6.2) that time oscillations of the pore pressure may occur for other time schemes. Associated to the Terzaghi's postulate, oscillations could appear also on the stress tensor, what can degrade the numerical convergence rate for elastoplastic or elastoviscoplastic constitutive laws.

Large strains and large displacements have been analysed for solid mechanics. When solid mechanics is coupled with pore pressure diffusion, the Darcy's fluid velocity and the balance equations have to be computed in the geometry of the current configuration, which is changing from one iteration to the other. Therefore a geometric coupling term appears in the iteration matrix when derivating the nodal water fluxes with respect to the nodal displacements. On the other hand, the solid and fluid specific weights have to be actualised taking into account the large strain process [BAR 98].

When using isoparametric finite elements, the shape functions for geometry and for pore pressure are identical. Let us consider for example a second order finite element. As the displacement field is of second order, the strain rate field is linear. For an elastic material, the effective stress tensor rate is then also linear. However the pore pressure field is quadratic. Then the Terzaghi's postulate mixes linear and quadratic field, which is not highly consistent. Some authors have then proposed to mix in one element quadratic shape functions for the geometry and linear shape functions for pore pressure. But then problems arrive with the large strain geometry evolution and with the choice of spatial integration points (1 or 4 Gauss points?).

Numerical locking problems may also appear for isoparametric finite element when the two phases material (water + soil) is quite incompressible, i.e. for very short time steps with respect with the fluid diffusion time scale. Specific elements have to be developed for such problems.

7.3.2.2. Thermo-hydro-mechanical coupling

The phenomena considered here (as for example for problems related to underground storage of nuclear waste disposals – [GEN 01b]) are much more complex as they associate multiphase fluid flow, hydromechanical coupling (section 7.3.2.1) and temperature effects. All the features described in the preceding section are to be considered here, associated to some new points. The total number of dof per node needed is 5 for a 2D problem (2 displacements, 2 fluid pore pressures and the temperature) and 6 for a 3D problem (3 displacements, 2 fluid pore pressures and the temperature).

Heat diffusion has to be modelled. Temperature variation affects fluid flow, by a modification of the fluid specific weight or viscosity. Moreover, if the two fluids concerned are a liquid and a gas (e.g. water and air), then equilibrium between the phases has to be modelled: dry air – vapour equilibrium.

Heat transfer is governed not only by conduction but also by advection by the liquid and gas movements. Similarly transfers of vapour and dry air in the gas phase are governed by diffusion and gradient of species density, but also by advection of the global gas movements. If the concerned geomaterials has a very low permeability (like clay for engineered barriers), the diffusion effects will predominate and advection doesn't necessitate specific formulation (section 7.2.7) [COL 02].

7.3.3. Finite element modelling: staggered approach

Monolithical approach of coupled phenomena implies identical space and time meshes for each phenomenon. This is not always possible, for various reasons. The coupled problems may have different numerical convergence properties, generally associated to different physical scales or non-linearities. For example, a coupled hydromechanical problem may need large time steps for the fluid diffusion problem, in order to allow in each step fluid diffusion along distance of the order of magnitude of the finite elements. In the same time, strong non-linearities may occur in solid mechanics behaviour (strong elastoplasticity changes, interface behaviour, strain localisation…) and then the numerical convergence needs short time – loading steps, which should be adapted automatically to the rate of convergence. Then it is quite impossible to obtain numerical convergence for identical time and space meshes.

Research teams of different physical and numerical culture have progressively developed different problems modelling. As an example, fluid flow has been largely developed using the finite difference method for hydrogeology problems including pollutant transport, and for oil reservoir engineering (section 7.2.1 and 7.2.3) taking multiphase fluid flow (oil, gas, condensate, water…) into account. Coupling such fluid flow with geomechanics in a monolithical approach would imply to implement

all the physical features already developed respectively in finite elements and finite differences codes. The global human effort would be very important.

Coupled problems are generally presenting a higher non-linearity level then uncoupled ones. Then inaccuracy in parameters or in the problem idealisation may cause degradations of the convergence performance.

How can we solve such problems and obtain a convincing solution? First of all, a good strategy would be to start with the uncoupled modelling of the leading process, and to try to obtain a first not too bad solution. Then one can add a first level of coupling and complexity, followed by a second one… until the full solution is obtained.

However such trick is not always sufficient. Staggered approaches may then give an interesting solution. In a staggered scheme, the different problems to be coupled are solved separately, with (depending on the cases) different space or time mesh, or different numerical codes. However, the coupling is ensured thanks to the transfer of information between the separated models at regular meeting points. This concept is summarised on the Figure 7.3. It allows theoretically coupling any models together.

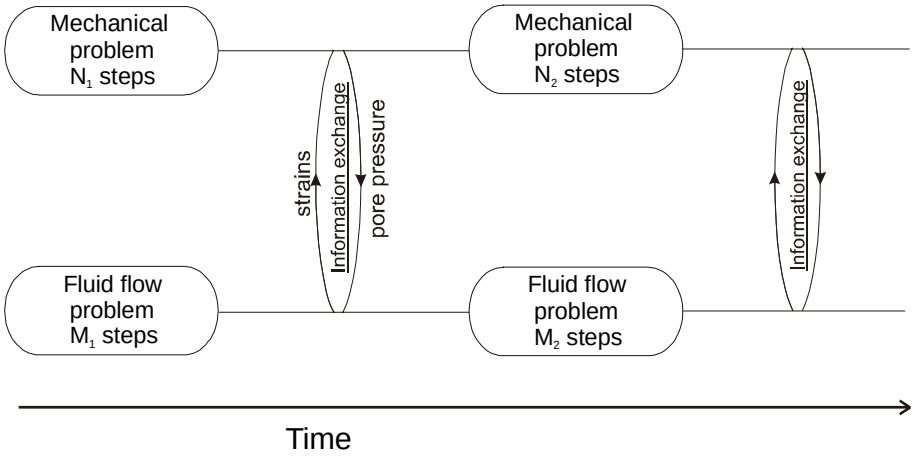

Figure 3. *Scheme of a staggered coupling*

When using different spatial meshes, or when coupling finite elements and finite differences codes, the transfer of information needs often an interpolation procedure, as the information to be exchanged are not defined at the points in the different meshes.

The accuracy of the coupling scheme will mainly depend on the information exchanges frequency (which is limited by the lower time step that can be used) and by the type of information exchanged. The stability and accuracy of the process has

been checked by different authors [TUR 93, ZIE 88, RAD 94]. It has been shown that a good choice of the information exchange may improve highly the procedure efficiency.

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