INTRODUCTION TO NUMERICAL MODELIZATION RELEVANT TO CONTINUOUS MEDIA
NUMERICAL METHODS COURSES
materials master

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Abstract

This course is a relatively short introduction to numerical computational methods relevant to continuous media for solving partial differential equations (PDE) problems. As the finite element method is by far the most widely used method at present, it naturally forms the major part of the course. However, other classical methods, such as the boundary element method, are described in some detail. It is essential to refer to more complete works to deepen these notions [14] [19] [20] [8] [13].

Keywords: computational methods, continuum media, spatial discretization, finite elements, finite volumes, finite differences, boundary element method, semi-analytical method

Contents

Foreword

This course is a modest introduction to numerical modeling in continuous media. It is more focused on pedagogy than on demonstrative rigour[1]. Only those details deemed essential by the author for a first approach are provided. It is recommended to refer to more complete works to deepen these concepts [14] [19] [20] [8], [13], etc. It has been more convenient for the author to illustrate this course with examples from thermomechanics, although the methods presented here cover all areas requiring the solution of PDEs in continuous media.

1. Introduction

1.1. Background

In scientific research it is often a question of

<u>describe and explain to predict</u>

Reliable prediction methods are therefore essential for the advancement of knowledge.

1.1.1. Typical problems

The problems encountered in continuous media generally concern diffusion, electrical or thermal conduction, fluid mechanics and solid mechanics. These problems can be *coupled* as for example :

+ diffusion of a fluid in a solid - the fluid content changing the properties of the solid,

+ self-heating of a solid due to mechanical loading - temperature changing mechanical properties,

+ interactions between fluid and structure such as the effect of swell on an oil platform - boundary conditions on the solid depend on the action of a fluid,

+ etc.

Problems can be of the steady state or transient type.

1.1.2. Status of numerical modelling among possible investigation methods

The methods of scientific investigation for the purpose of increasing knowledge are essentially :

+ experimental or observational campaigns and data processing,

+ analytical models,

+ numerical models.

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[1]Although pedagogy most probably requires a lot of rigour, but a reasonable compromise must be made.

These methods complement each other since it is necessary to validate the prediction tools. The diagram in Fig. 1 illustrates the different possible interactions between these methods. For each problem and its specificities,
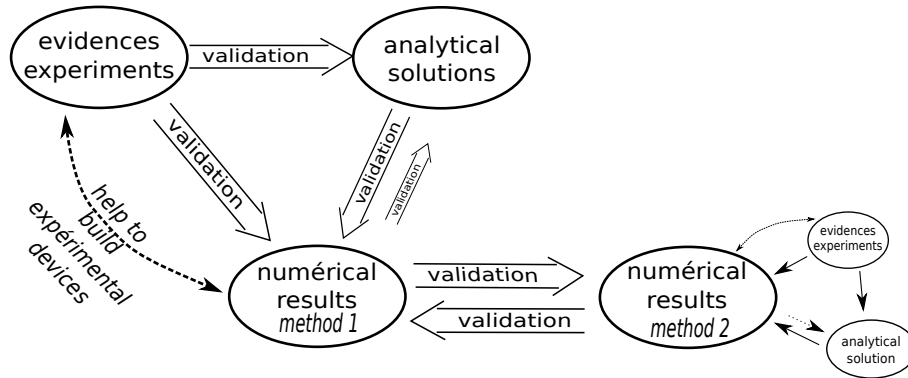
Figure 1: Possible investigation methods and validations.

the situation must be analysed. Depending on the discipline, some choices may be more frequents than others. Let us mention some criteria of choice to develop a scientific approach :

+ what may make the analytical result unattainable within a given time frame :

= complex, non-linear constitutive equations, ...

= complex boundary conditions :

- complex geometry,

- complex boundary conditions.

+ which may make the experimental result unreachable within a given time :

= coupled phenomena with difficult decoupling, ...

= cost ($€$, \$, ...)

= duration

= risk

= possibility of experimentation (science of the earth and the universe, medicine, ...)

Numerical models can then overcome these difficulties. They can eventually validate each other, usually partially for the common problems they can address. However, to allow for bilateral validation, they must be sufficiently different conceptually.

1.2. Classical constitutive equations

Partial differential equations *(PDEs)* are used in the formulations of the laws.

1.2.1. Balances and conservation

The expressions of the vector operators used here can be found in Appendix A. Here are the most commonly encountered conservation or equilibrium equations:

This equation translates the dynamic equilibrium in deformable solid mechanics:

$$\overrightarrow{div}(\underline{\sigma}) + \overrightarrow{f} - \rho\overrightarrow{\gamma} = \overrightarrow{0} \tag{1}$$

where $\underline{\sigma}$ is the Cauchy stress tensor ("real stresses"), $\overrightarrow{f}$ are the body forces (for instance $\overrightarrow{f} = \rho\overrightarrow{g}$ where $\overrightarrow{g}$ is the acceleration of gravity and ρ the density of the material) and $\overrightarrow{\gamma}$ the acceleration of matter.

This equation reflects heat conduction and thermal equilibrium:

$$div(\overrightarrow{q}) - c\frac{\partial T}{\partial t} = 0 \tag{2}$$

where $\overrightarrow{q}$ denotes the heat flux, c the mass heat, T the temperature and t the time. The equation for the conduction of electricity is analogous.

Among the conservation equations are those called *Navier-Stokes equations*. For example, for viscous compressible fluids conservation of mass implies:

$$\frac{\partial \rho}{\partial t} + \rho div(\overrightarrow{V}) = 0 \tag{3}$$

and the conservation of momentum implies:

$$\rho\frac{\partial \overrightarrow{V}}{\partial t} = \rho\overrightarrow{f} - \overrightarrow{grad}(p - \frac{\eta}{3}div(\overrightarrow{V})) + \eta\nabla^2(\overrightarrow{V}) \tag{4}$$

where $\overrightarrow{V}$ denotes the velocity of the fluid, ρ its density, η its viscosity, $\overrightarrow{f}$ the volume forces, p the pressure and t the time. For a fluid, incompressibility is expressed by $div(\overrightarrow{V}) = 0$ where $\overrightarrow{V}$ is the velocity of the fluid. For viscous incompressible fluids, the Navier-Stokes equation for conservation of momentum thus becomes $\rho\frac{\partial \overrightarrow{V}}{\partial t} = \rho\overrightarrow{f} - \overrightarrow{grad}(p) + \eta\nabla^2(\overrightarrow{V})$.

etc.

1.2.2. Behaviour laws

Behaviour laws or behaviour equations establish an observed link between stresses and their effects.

$\underline{\sigma} = \underline{\underline{C}}\,\underline{\epsilon}$ denotes linear elastic behaviour in solid mechanics. $\underline{\sigma}$ designates the stress tensor, $\underline{\epsilon}$ the strain tensor and $\underline{\underline{C}}$ the compliance tensor. The latter is

of order 4 since stresses and strains are tensors of order 2 and it can describe anisotropic behaviour.

The equation $div(\overrightarrow{q}) = -\lambda\,\overrightarrow{grad}(T)$ is called *Fourier's law* and expresses the thermal conduction. As $div(\overrightarrow{grad})() = \triangle()$, equation 2 becomes $lambda \triangle (T) + c\frac{partialT}{partialt} = 0$.

$dev(\underline{\sigma}) = \eta\,dev(\underline{\dot{\epsilon}})$ translates the behaviour of a *newtonian* fluid, i.e. its viscosity η does not depend on the shear rate $\dot{\epsilon}\partial t$.

etc.

1.3. Boundary conditions

The boundary conditions deal with the limits of the spatial domain concerned and the temporal domain concerned.

1.3.1. Spatial boundary conditions

Conditions can be mixed in the same area.

$\underline{\sigma}.\overrightarrow{n} = \overrightarrow{T}$ xpresses oriented surface force conditions, in N/m^2, where $\overrightarrow{n}$ denotes the outgoing surface normal and $\overrightarrow{T}$ the prescribed pressure condition.

$\overrightarrow{q}.\overrightarrow{n} = h$ defines an outgoing or incoming heat flow.

$\overrightarrow{U} = \overrightarrow{U_{CL}}$ defines a given displacement. $\overrightarrow{V} = \overrightarrow{V_{CL}}$ defines a given speed.

etc.

1.3.2. Time boundary conditions

The initial conditions describe the imposed states and evolutions as a function of time.

$\overrightarrow{F}(t) = \overrightarrow{F_0}$ *at* $t = 0$ expresses for example the initial value of a force.

$\overrightarrow{U}(t) = \overrightarrow{U_0}$ *at* $t = 0$ expresses for example the initial value of a displacement. $\overrightarrow{U}(t) = \overrightarrow{U_0}\,sin(\omega t)$ expresses, for example, that the evolution of the displacement is harmonic with pulsation ω and is equal to 0 at $t = 0$.

$\overrightarrow{V}(t) = \overrightarrow{V_0}$ *at* $t = 0$, expresses for example the initial value of a speed.

$\ddot{U}(t) = \overrightarrow{0}$, expresses for example that the material acceleration is zero at

the start of the calculation.

$T(t) = T_0$ *at* $t = 0$, expresses for example that the initial temperature is T_0.

etc.

For further information, see for example [16], [5], [12], [18] et [11].

2. General methods of resolution

NB. This is only a list of entry points with some key words. More information can be found for example in [12] [14] [13].

We are looking for the best possible solution $\overrightarrow{\tilde{U}}(P)$, where P designates a point of coordinates (x, y, z), i.e. the solution which is the closest possible to the exact solution designated by $\overrightarrow{U}(P)$, this last one not necessarily being known. The vector $\overrightarrow{U}(P)$ can have several components. For example $\overrightarrow{U}(P) = (u_x, u_y, u_z, T)_P$ if we are looking for the displacement according to $(\overrightarrow{x}, \overrightarrow{y}, \overrightarrow{z})$ and the temperature T of point P.

In a domain $\mathscr{D}$ we give ourselves a set of functions $\phi_i(P)$. This set is called a *"functional base"*. These functions must be continuous, respect the boundary conditions and satisfy completeness. They can also have various properties according to the imperatives and conveniences of use such as derivability, normality, orthogonality, etc. Polynomials, Taylor series and harmonic functions are often used. The problem now comes down to finding the coefficients a_i which best satisfy a given criterion ($\overrightarrow{\tilde{U}}(P)$ as close as possible to $\overrightarrow{U}(P)$ in the sense of the criterion we have given ourselves) and such that:

$$\tilde{u}_x(P) = \sum_{i=1}^{N} a_{xi} \ \phi_i(P) \tag{5}$$

of course the same applies to the other components of the $\overrightarrow{U}(P)$, $\tilde{u}_y(P) = \sum_{i=1}^{N} a_{yi} \ \phi_i(P)$, $\tilde{u}_z(P) = \sum_{i=1}^{N} a_{zi} \ \phi_i(P)$ and $\tilde{T}(P) = \sum_{i=1}^{N} a_{Ti} \ \phi_i(P)$. The $\mathscr{D}$ domain can be discretised into subdomains as in the finite element method. It is then a question of obtaining a linear system of equations where the coefficients a_{qi} will be the unknowns, q designating the component (x, y, z or T...) and i the coefficient of the function ϕ_i. It is obvious that the ϕ_i-functions must be able to describe the fields adequately, starting with a uniform field. A common feature of various approximation methods is to introduce an error function and then to minimise this error function as best as possible, denoted by $err(P) = E(\overrightarrow{U}(P))$. The error is integrated on the domain $\mathscr{D}$ and we give ourselves a weighting w_i. As we wish to obtain the minimal error, we try to satisfy:

$$\int_{\mathscr{D}} err(P)\, w_i(P)\, dv = 0 \tag{6}$$

This gives an equation and we have several unknowns a_{qi}. We must therefore give ourselves several suitable weighting functions w_i to obtain a system where there are as many equations as there are unknowns.

2.1. Galerkin's method

Galerkin's method was proposed around 1915. It consists in using as a weight the ϕ_i function itself, i.e. $w_i(P) = \phi_i(P)$. As it can be shown that the error committed is orthogonal to the approximation subspaces, we can write that:

$$\int_{\mathscr{D}} err(P)\, \phi_i(P)\, dv = 0 \tag{7}$$

This method provides a priori as many equations as functions ϕ_i.

2.2. Miklin's method

Miklin's method consists of finding the solution to a problem by least squares.

$$\frac{\partial}{\partial a_{qi}} \int_{\mathscr{D}} err^2(P)\, dv = \int_{\mathscr{D}} err(P) \frac{\partial err(P)}{\partial a_{qi}} dv = 0 \tag{8}$$

this corresponds to posing $w_i(P) = \frac{partialerr(P)}{\partial a_i}$. This method provides as many equations as there are coefficients a_{qi}.

2.3. Collocation method

The point collocation method consists of finding the solution of a problem that passes exactly through given points P_i.

$$\int_{\mathscr{D}} err(M)\delta(\overrightarrow{OM} - \overrightarrow{OP_i})\, dv = err(P_i) = 0 \tag{9}$$

where $\delta()$ denotes the Dirac function. This amounts to posing $w_i(P) = \delta(\overrightarrow{OM} - \overrightarrow{OP_i})$. This method provides as many equations as there are P_i points. An example of the collocation method can be found in [13] applied to elasticity for a crack in a plane infinite medium.

2.4. Ritz method

The Ritz method was proposed around 1909. It consists in finding the solution of a problem in its variational form, i.e. $\delta V = 0$ where $V(\overrightarrow{U}) = \int_{\mathscr{D}} \mathscr{L}(\overrightarrow{U}, \overrightarrow{U}', \overrightarrow{U}'', ...)$ where $\mathscr{L}$ designates the Lagrangian of the system. The equilibrium position is sought by looking for the stationarity which is expressed by:

$$\frac{\partial \mathscr{L}(\overrightarrow{U})}{\partial a_{qi}} = 0 \tag{10}$$

This amounts to posing $w_i = 1$ and $err(P) = \mathscr{L}(P)$. This method provides as many equations as there are coefficients a_{qi}.

NB. In some cases, e.g. elasticity functions, the Ritz and Galerkin methods are equivalent.

2.5. Meshless method, diffuse element, ...

Methods based on unknown nodal values but without meshing, (*mesh-less, diffuse element method, element-free Galerkin method, ...*), exist and sometimes represent an interesting alternative for example to the finite element method. I recommend the reading of https://pdfcoffee.com/meshlesspdf-pdf-free.html to discover these methods, advantages and disadvantages.

3. Finite element method

3.1. Nodes, elements and connectivity

The *nodes* are the points in space where we want to evaluate unknowns (i, j, k, l, ... in lower case in Fig. 2). The nodes are used as support for the *finite elements*. A finite element (C, D, E, F, ... in upper case in Fig. 2) is a spatial domain in which the values of the unknowns are interpolated from the nodal values. The whole constitutes a mesh of the domain $\mathscr{D}$. A mesh can consist of several different types of elements. The *connectivities*
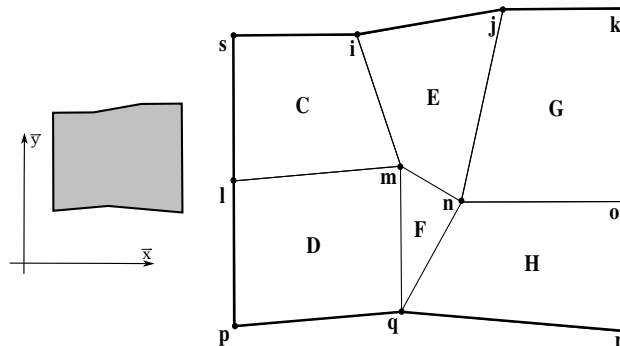
Figure 2: Two-dimensional spatial discretization of a surface. The mesh is composed of 5 quadrilaterals with four nodes and 1 triangle with 3 nodes.

table describes the organisation of the mesh. The order of the nodes must respect the convention chosen by the software, for example the element E is described by turning clockwise by (i, j, n, m) and not (i, j, m, n) in order to be able to define a quadrilateral properly and easily its interior and exterior. The elements can be one-dimensional, two-dimensional or three-dimensional and have different numbers of nodes for the same geometrical shape as shown in Fig. 3.

element	node 1	node 2	node 3	node 4
C	s	i	m	l
D	l	m	q	p
E	i	j	n	m
G	k	o	n	j
H	n	o	r	q
F	m	n	q	

Table 1: Connectivity table for the mesh of Fig. 2.

Figure 3: Examples of elements: beam with 2 nodes, triangles with 3 and 6 nodes, quadrilaterals with 4, 8 and 9 nodes, tetrahedrons with 4 and 10 nodes, cubes with 8 and 20 nodes.
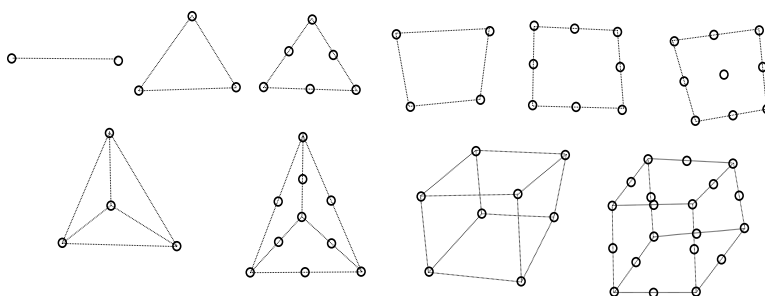
3.2. Interpolation fonction

The *interpolation function*, sometimes referred to as *shape function*, is used to describe the evolution of a variable within the element knowing only the value it takes at the nodes. For example, for a quadrilateral with 4 nodes, if $q(a, b)$ denotes the variable with $a \in [-1, +1]$ and $b \in [-1, +1]$, $q_i = q(-1, +1)$, $q_j = (+1, +1)$, $q_n = q(+1, -1)$ and $q_m = q(-1, -1)$ denote respectively the value of this variable at nodes i, j, n, and m then an interpolation function can be defined by:

$$q(a, b) = \frac{q_i \ (1 - a)(1 + b)}{4} + \frac{q_j \ (1 + a)(1 + b)}{4}$$

$$+ \frac{q_n \ (1 + a)(1 - b)}{4} + \frac{q_m \ (1 - a)(1 - b)}{4} \tag{11}$$

The interpolation functions must:
- allow simple calculations,
- allow to represent a uniform field,
- have properties such as continuity and derivability.

3.3. Real space, parametric space

The interpolation function is defined in the parameter space. The real space can have any form as shown in Fig. 4. Let us denote by $\mathscr{Q}(x, y)$

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the function corresponding to $q(a, b)$. It is then a question of being able to describe the evolutions of the variable q in the real space of different form. To do this, we can use the same interpolation function for the spatial positions and the evolution of the variable q. The element is then *isoparametric* and $q(a, b) = \mathcal{Q}(x(a, b), y(a, b))$ leads to:

$$x(a, b) = \frac{x_i \ (1-a)(1+b)}{4} + \frac{x_j \ (1+a)(1+b)}{4}$$

$$+ \frac{x_n \ (1+a)(1-b)}{4} + \frac{x_m \ (1-a)(1-b)}{4} \tag{12}$$

where (x_i, y_i), (x_j, y_j), (x_m, y_m) and (x_n, y_n) are respectively the coordinates of nodes i, j, m and n. Similarly:

$$y(a, b) = \frac{y_i \ (1-a)(1+b)}{4} + \frac{y_j \ (1+a)(1+b)}{4}$$

$$+ \frac{y_n \ (1+a)(1-b)}{4} + \frac{y_m \ (1-a)(1-b)}{4}$$
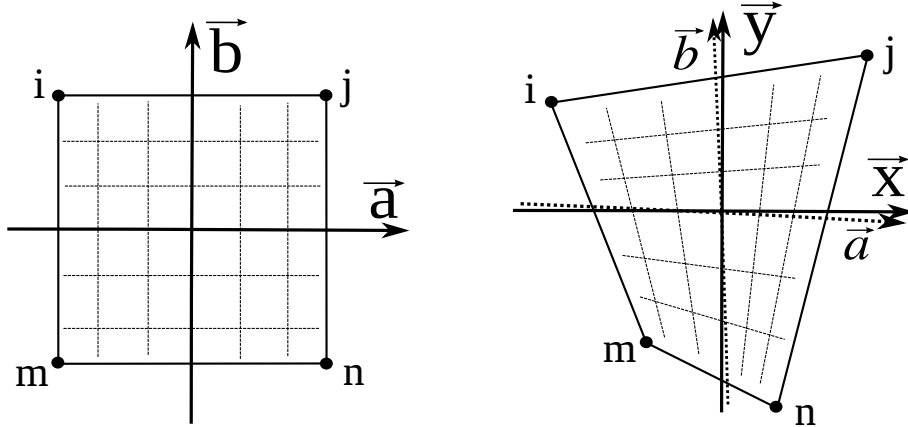
Figure 4: Parametric space (left) and real space (right).

In order to solve PDE's, it is necessary to differentiate in parametric space in order to follow the evolutions in real space corresponding to the evolutions in parametric space and vice versa. It is therefore necessary to calculate $d\mathcal{Q}(x, y) = \frac{\partial \mathcal{Q}}{\partial x} dx + \frac{\partial \mathcal{Q}}{\partial y} dy$. By expanding, we obtain:

$$d\mathcal{Q}(x(a, b), y(a, b)) = \frac{\partial \mathcal{Q}}{\partial x}\left(\frac{\partial x}{\partial a} da + \frac{\partial x}{\partial b} db\right) + \frac{\partial \mathcal{Q}}{\partial y}\left(\frac{\partial y}{\partial a} da + \frac{\partial y}{\partial b} db\right)$$

$$d\mathcal{Q}(x(a, b), y(a, b)) = \left(\frac{\partial \mathcal{Q}}{\partial x}\frac{\partial x}{\partial a} + \frac{\partial \mathcal{Q}}{\partial y}\frac{\partial y}{\partial a}\right) da + \left(\frac{\partial \mathcal{Q}}{\partial x}\frac{\partial x}{\partial b} + \frac{\partial \mathcal{Q}}{\partial y}\frac{\partial y}{\partial b}\right) db$$

et

$$\begin{bmatrix} \frac{\partial \mathcal{Q}}{\partial a} \\ \frac{\partial \mathcal{Q}}{\partial b} \end{bmatrix} = \begin{bmatrix} \frac{\partial x}{\partial a} & \frac{\partial y}{\partial a} \\ \frac{\partial x}{\partial b} & \frac{\partial y}{\partial b} \end{bmatrix} \begin{bmatrix} \frac{\partial \mathcal{Q}}{\partial x} \\ \frac{\partial \mathcal{Q}}{\partial y} \end{bmatrix} = \mathbf{J} \begin{bmatrix} \frac{\partial \mathcal{Q}}{\partial x} \\ \frac{\partial \mathcal{Q}}{\partial y} \end{bmatrix}$$

$\mathbf{J}$ is called the Jacobian matrix of the transformation. Its inverse is easily identified.

$$\mathbf{J} = \begin{bmatrix} \frac{\partial x}{\partial a} & \frac{\partial y}{\partial a} \\ \frac{\partial x}{\partial b} & \frac{\partial y}{\partial b} \end{bmatrix} \qquad \mathbf{J}^{-1} = \begin{bmatrix} \frac{\partial a}{\partial x} & \frac{\partial b}{\partial x} \\ \frac{\partial a}{\partial y} & \frac{\partial b}{\partial y} \end{bmatrix} \tag{13}$$

Since $\mathcal{Q}(x(a,b), y(a,b)) = q(a,b)$:

$$\overrightarrow{grad}(q) = \begin{bmatrix} \frac{\partial q}{\partial a} \\ \frac{\partial q}{\partial b} \end{bmatrix} = \begin{bmatrix} \frac{\partial q}{\partial x}\frac{\partial x}{\partial a} + \frac{\partial q}{\partial y}\frac{\partial y}{\partial a} \\ \frac{\partial q}{\partial x}\frac{\partial x}{\partial b} + \frac{\partial q}{\partial y}\frac{\partial y}{\partial b} \end{bmatrix} = \begin{bmatrix} \frac{\partial x}{\partial a} & \frac{\partial y}{\partial a} \\ \frac{\partial x}{\partial b} & \frac{\partial y}{\partial b} \end{bmatrix} \begin{bmatrix} \frac{\partial \mathcal{Q}}{\partial x} \\ \frac{\partial \mathcal{Q}}{\partial y} \end{bmatrix} = \mathbf{J}\,\overrightarrow{grad}(\mathcal{Q}) \tag{14}$$

and vice versa $\overrightarrow{grad}(\mathcal{Q}) = \mathbf{J}^{-1}\overrightarrow{grad}(q)$.

3.4. Isoparametric element and jacobian matrix

In order to solve PDEs, it is necessary to differentiate in parametric space in order to follow the evolutions in real space corresponding to the evolutions in parametric space. It is therefore necessary to calculate $dx(a,b) = \frac{\partial x}{\partial a}da + \frac{\partial x}{\partial b}db$ et $dy(a,b) = \frac{\partial y}{\partial a}da + \frac{\partial y}{\partial b}db$:

$$\begin{bmatrix} dx \\ dy \end{bmatrix} = \begin{bmatrix} \frac{\partial x}{\partial a} & \frac{\partial x}{\partial b} \\ \frac{\partial y}{\partial a} & \frac{\partial y}{\partial b} \end{bmatrix} \begin{bmatrix} da \\ db \end{bmatrix} = \mathbf{J}^T \begin{bmatrix} da \\ db \end{bmatrix}$$

$$dx(a,b) = \frac{x_i\left[-(1+b)da + (1-a)db\right]}{4} + \frac{x_j\left[(1+b)da + (1+a)db\right]}{4}$$
$$+ \frac{x_n\left[(1-b)da - (1+a)db\right]}{4} + \frac{x_m\left[-(1-b)da - (1-a)db\right]}{4} \tag{15}$$

and

$$dy(a,b) = \frac{y_i\left[-(1+b)da + (1-a)db\right]}{4} + \frac{y_j\left[(1+b)da + (1+a)db\right]}{4}$$
$$+ \frac{y_n\left[(1-b)da - (1+a)db\right]}{4} + \frac{y_m\left[-(1-b)da - (1-a)db\right]}{4}$$

This makes it possible to calculate the Jacobian matrix in the case of the chosen interpolation:

$$J_{11} = \frac{\partial x}{\partial a} = [x_j - x_i + x_n - x_m + b(x_j - x_i + x_n - x_m)]/4$$

$$J_{12} = \frac{\partial y}{\partial a} = [y_j - y_i + y_n - y_m + b(y_j - y_i - y_n + y_m)]/4$$

$$J_{21} = \frac{\partial x}{\partial b} = [x_i + x_j - x_n - x_m + a(x_j - x_i + x_n - x_m)]/4$$

$$J_{22} = \frac{\partial y}{\partial b} = [y_i + y_j - y_n - y_m + a(y_j - y_i - y_n + y_m)]/4$$

Conversely, we get:

$$\begin{bmatrix} da \\ db \end{bmatrix} = \begin{bmatrix} \frac{\partial a}{\partial x} & \frac{\partial a}{\partial y} \\ \frac{\partial b}{\partial x} & \frac{\partial b}{\partial y} \end{bmatrix} \begin{bmatrix} dx \\ dy \end{bmatrix} = (\mathbf{J}^{-1})^T \begin{bmatrix} dx \\ dy \end{bmatrix} \tag{16}$$

3.5. Gradient of an interpolated variable computation

3.5.1. General case

In order to solve the PDEs, it is necessary to calculate, among other things, the gradients of the variables, for example the temperature in order to know the flux or the displacements in order to know the deformations. For example, let us calculate the deformations for a plane problem in the case of small perturbations hypotheses (S. P. H.).[2] If the displacement according to $\overrightarrow{x}$, is designated by u then it comes: $\epsilon_{xx} = \frac{\partial u}{\partial x} = \frac{\partial u}{\partial a}\frac{\partial a}{\partial x} + \frac{\partial u}{\partial b}\frac{\partial b}{\partial x}$ where ϵ_{xx} represents the longitudinal strain according to $\overrightarrow{x}$. Similarly, ϵ_{yy} represents the longitudinal strain according to v and the displacement along $\overrightarrow{y}$, $\epsilon_{yy} = \frac{\partial v}{\partial y} = \frac{\partial v}{\partial a}\frac{\partial a}{\partial x} + \frac{\partial v}{\partial b}\frac{\partial b}{\partial x}$. The shear strain, referred to as $\epsilon_{xy} = \frac{1}{2}\gamma_{xy}$, is given by $\epsilon_{xy} = \frac{1}{2}(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x})$ and is calculated in a similar way, i. e. $\gamma_{xy} = 2\epsilon_{xy} = \frac{\partial u}{\partial a}\frac{\partial a}{\partial y} + \frac{\partial u}{\partial b}\frac{\partial b}{\partial y} + \frac{\partial v}{\partial a}\frac{\partial a}{\partial x} + \frac{\partial v}{\partial b}\frac{\partial b}{\partial x}$. Note that these equations show the terms of $\mathbf{J}^{-1}$. Let us return to the q notation of the interpolation where q plays the role of the displacement u or the displacement v in an elasticity problem. The derivatives of q, the latter being represented by the interpolation function, in the parameter space gives:

$$\frac{\partial q(a,b)}{\partial a} = \frac{q_i\,(-1-b)}{4} + \frac{q_j\,(1+b)}{4} + \frac{q_n\,(1-b)}{4} + \frac{q_m\,(-1+b)}{4}$$

$$\frac{\partial q(a,b)}{\partial b} = \frac{q_i\,(1-a)}{4} + \frac{q_j\,(1+a)}{4} + \frac{q_n\,(-1-a)}{4} + \frac{q_m\,(-1+a)}{4}$$

which can be put in the form:

$$\begin{bmatrix} \frac{\partial q(a,b)}{\partial a} \\ \frac{\partial q(a,b)}{\partial b} \end{bmatrix} = \begin{bmatrix} N_{i,a} & N_{j,a} & N_{n,a} & N_{m,a} \\ N_{i,b} & N_{j,b} & N_{n,b} & N_{m,b} \end{bmatrix}_{(a,b)} \begin{bmatrix} q_i \\ q_j \\ q_n \\ q_m \end{bmatrix} \tag{17}$$

By combining 13 and 17 we finally obtain:

$$\overrightarrow{grad}(\mathcal{Q}) = \begin{bmatrix} \frac{\partial \mathcal{Q}}{\partial x} \\ \frac{\partial \mathcal{Q}}{\partial y} \end{bmatrix} = \begin{bmatrix} J_{11}^{-1} & J_{12}^{-1} \\ J_{21}^{-1} & J_{22}^{-1} \end{bmatrix} \begin{bmatrix} N_{i,a} & N_{j,a} & N_{n,a} & N_{m,a} \\ N_{i,b} & N_{j,b} & N_{n,b} & N_{m,b} \end{bmatrix} \begin{bmatrix} q_i \\ q_j \\ q_n \\ q_m \end{bmatrix} \tag{18}$$

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[2]SPH stipulate that the displacements are small and the strains are small.

By replacing $\mathcal{Q}$ by u and then by v, the two components of displacement in the plane, we can calculate the deformations. In the same way, $\mathcal{Q}$ can be replaced by T, the temperature, for the calculation of heat flux, etc. If the mechanical behaviour, the elastic constants for example, depends on the temperature for a thermomechanical model then there will necessarily be 3 unknowns per node, u, v and T and the calculation will be said to be coupled thermomechanical.

3.5.2. The case of plane elasticity: example of a plane problem with two unknown components

For a calculation of deformations in the plane, the unknowns associated with the element considered here - a quadrilateral with four nodes - are therefore eight in number: $u_i, u_j, u_n, u_m, v_i, v_j, v_n$ and v_m. For the whole problem, a vector will be constituted by all the unknowns, essentially[3], the displacements according to $\overrightarrow{x}$ and $\overrightarrow{y}$ at the nodes. Let us therefore consider the vector of unknowns and deduce the deformations. The partial derivatives in the parameter space are given by:

$$
\begin{bmatrix} \frac{\partial u}{\partial a} \\ \frac{\partial u}{\partial b} \\ \frac{\partial v}{\partial a} \\ \frac{\partial v}{\partial b} \end{bmatrix} = \begin{bmatrix} N_{i,a} & N_{j,a} & N_{n,a} & N_{m,a} & 0 & 0 & 0 & 0 \\ N_{i,b} & N_{j,b} & N_{n,b} & N_{m,b} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & N_{i,a} & N_{j,a} & N_{n,a} & N_{m,a} \\ 0 & 0 & 0 & 0 & N_{i,b} & N_{j,b} & N_{n,b} & N_{m,b} \end{bmatrix} \begin{bmatrix} u_i \\ u_j \\ u_n \\ u_m \\ v_i \\ v_j \\ v_n \\ v_m \end{bmatrix} \quad (19)
$$

The strains in real space are given by:

$$
\begin{bmatrix} \frac{\partial u}{\partial x} \\ \frac{\partial u}{\partial y} \\ \frac{\partial v}{\partial x} \\ \frac{\partial v}{\partial y} \end{bmatrix} = \begin{bmatrix} J_{11}^{-1} & J_{12}^{-1} & 0 & 0 \\ J_{21}^{-1} & J_{22}^{-1} & 0 & 0 \\ 0 & 0 & J_{11}^{-1} & J_{12}^{-1} \\ 0 & 0 & J_{21}^{-1} & J_{22}^{-1} \end{bmatrix} \begin{bmatrix} \frac{\partial u}{\partial a} \\ \frac{\partial u}{\partial b} \\ \frac{\partial v}{\partial a} \\ \frac{\partial v}{\partial b} \end{bmatrix} \quad (20)
$$

The tensor of deformations in the plane is given by:

$$
\begin{bmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ 2\epsilon_{xy} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial u}{\partial x} \\ \frac{\partial u}{\partial y} \\ \frac{\partial v}{\partial x} \\ \frac{\partial v}{\partial y} \end{bmatrix} \quad (21)
$$

Recall that $\underline{\underline{\epsilon}}$ is symmetric by construction and that $2\epsilon_{xy} = \gamma_{xy}$. By associating 1 to $\overrightarrow{x} \otimes \overrightarrow{x}$ and 2 to $\overrightarrow{y} \otimes \overrightarrow{y}$ and 3 to $\overrightarrow{x} \otimes \overrightarrow{y}$, and renaming the 8

---

[3]We will see later how to deal with an unknown force, such as a support reaction, associated with a known displacement.

unknowns q_r we can put the equations 19, 20 and 21 in the form:

$$\begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \end{bmatrix} = \begin{bmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ 2\epsilon_{xy} \end{bmatrix} = \mathbf{B} \begin{bmatrix} u_i \\ u_j \\ u_n \\ u_m \\ v_i \\ v_j \\ v_n \\ v_m \end{bmatrix} = \mathbf{B} \begin{bmatrix} q_1 \\ q_2 \\ q_3 \\ q_4 \\ q_5 \\ q_6 \\ q_7 \\ q_8 \end{bmatrix}$$

which defines the matrix $[\mathbf{B}]$ that can be more easily manipulated in the form:

$$\epsilon_g = \sum_{r=1}^{8} B_{gr} \, q_r \tag{22}$$

with

$$[\mathbf{B}] = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix} \begin{bmatrix} J_{11}^{-1} & J_{12}^{-1} & 0 & 0 \\ J_{21}^{-1} & J_{22}^{-1} & 0 & 0 \\ 0 & 0 & J_{11}^{-1} & J_{12}^{-1} \\ 0 & 0 & J_{21}^{-1} & J_{22}^{-1} \end{bmatrix} \begin{bmatrix} N_{i,a} & N_{j,a} & N_{n,a} & N_{m,a} & 0 & 0 & 0 & 0 \\ N_{i,b} & N_{j,b} & N_{n,b} & N_{m,b} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & N_{i,a} & N_{j,a} & N_{n,a} & N_{m,a} \\ 0 & 0 & 0 & 0 & N_{i,b} & N_{j,b} & N_{n,b} & N_{m,b} \end{bmatrix}$$

3.6. Use of a law of behaviour: example of Hooke's law

The next step is to use a law of behaviour. Indeed, to satisfy the conditions of equilibrium of mechanics, it is necessary to calculate the forces whose sum must cancel out. These forces are induced in the material by the strains. In the case of linear elasticity, Hooke's law links deformations to stresses:

$$\sigma_1 = \sigma_{xx} = 2\mu\epsilon_{xx} + \lambda(\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz})$$

$$\sigma_2 = \sigma_{yy} = 2\mu\epsilon_{yy} + \lambda(\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz})$$

$$\sigma_3 = \sigma_{xy} = 2\mu\epsilon_{xy} \tag{23}$$

where λ and μ are material parameters called Lame coefficients. Recall that the stress and strain tensors are symmetrical, i. e. $\sigma_{xy} = \sigma_{yx}$, etc. For a plane problem $\sigma_{xz} = 0$, $\sigma_{yz} = 0$, $\epsilon_{xz} = 0$ and $\epsilon_{yz} = 0$. In the $\overrightarrow{z}$ direction two possibilities exist:

$$\sigma_{zz} = 0 \ in \ plane \ stresses \ (P.Stre.)$$

or

$$\epsilon_{zz} = 0 \ en \ plane \ strains \ (P.Stra.)$$

ϵ_{zz} or σ_{zz} as the case may be will be deduced from $\sigma_{zz} = 2\mu\epsilon_{zz} + \lambda(\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz})$. More details on plane elasticity problems, in particular on the admissibility conditions of the plane stress hypothesis, can be found in [13] and [7]. If for our example we place ourselves in plane stress then $2\mu\epsilon_{zz} +$

$\lambda(\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}) = 0$ from which $\epsilon_{zz} = \frac{-\lambda}{\lambda+2\mu}(\epsilon_{xx} + \epsilon_{yy})$ or again with the new notation $\epsilon_{zz} = \frac{-\lambda}{\lambda+2\mu}(\epsilon_1 + \epsilon_2)$.

$$\sigma_1 = (\lambda + 2\mu - \frac{\lambda^2}{\lambda + 2\mu})\epsilon_1 + (\lambda - \frac{\lambda^2}{\lambda + 2\mu})\epsilon_2$$

$$\sigma_2 = (\lambda + 2\mu - \frac{\lambda^2}{\lambda + 2\mu})\epsilon_2 + (\lambda - \frac{\lambda^2}{\lambda + 2\mu})\epsilon_1$$

$$\sigma_3 = \mu\epsilon_3$$

The matrix of elastic compliances depends only on the material, here the matrix C takes into account the condition of plane stresses which is a structural condition. The matrix **C** is thus not rigorously the matrix of compliances of the material but rather a matrix of the type of rigidity. To call it a compliance matrix is an abuse of language. **C** which in the case of plane deformations takes the form:

$$\begin{bmatrix}\sigma_1 \\ \sigma_2 \\ \sigma_3\end{bmatrix} = \begin{bmatrix} \lambda + 2\mu - \frac{\lambda^2}{\lambda+2\mu} & \lambda - \frac{\lambda^2}{\lambda+2\mu} & 0 \\ \lambda - \frac{\lambda^2}{\lambda+2\mu} & \lambda + 2\mu - \frac{\lambda^2}{\lambda+2\mu} & 0 \\ 0 & 0 & 2\mu \end{bmatrix} \begin{bmatrix}\epsilon_1 \\ \epsilon_2 \\ \epsilon_3\end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} \\ C_{21} & C_{22} & C_{23} \\ C_{31} & C_{32} & C_{33} \end{bmatrix}\begin{bmatrix}\epsilon_1 \\ \epsilon_2 \\ \epsilon_3\end{bmatrix}$$

such that:

$$\sigma_p = \sum_{q=1}^{3} C_{pg}\ \epsilon_g = \sum_{g=1}^{3}\sum_{r=1}^{8} C_{pg}\ B_{gr}\ q_r \tag{24}$$

3.7. Use of an equilibrium principle: example of static equilibrium

There are several ways to approach this notion. One can use energy approaches such as the virtual work theorem or principle[4]. In the quasi-static regime and in the absence of volume force the "principle" of virtual works is expressed as: $\int\int_{\partial\mathscr{D}} \overrightarrow{T}\overrightarrow{D^*}ds - \int\int\int_{\mathscr{D}} \underline{\sigma} : \underline{\epsilon}(\overrightarrow{D^*})dv = 0$, where $\mathscr{D}$ is the domain and $\partial\mathscr{D}$ its surface on which stress boundary conditions $\overrightarrow{T} = \underline{\sigma}\overrightarrow{n}$ or in displacements $\overrightarrow{D^*}$ can be imposed, $\underline{\sigma}$ being a statically admissible stress field, $\overrightarrow{n}$ the outgoing surface normal and $\overrightarrow{D^*}$ a kinematically admissible displacement field. In our case, $\overrightarrow{T}$ and $\overrightarrow{D^*}$ are associated, i. e. $\overrightarrow{D^*} = \overrightarrow{D}$ and $\underline{\sigma} = \mathbf{C}\underline{\epsilon}(\overrightarrow{D})$. A more common version of the virtual work "principle" is to consider increases in strain energy $\int\int\int_{\mathscr{D}} \underline{\sigma} : \underline{\epsilon}(\overrightarrow{D})dv$ and the work of external forces $\int\int_{\partial\mathscr{D}} \overrightarrow{T}\overrightarrow{D}ds$ and to write stationarity in a variational approach using the extremum principle: $\delta\int\int_{\partial\mathscr{D}} \overrightarrow{T}\overrightarrow{D}ds = \delta\int\int\int_{\mathscr{D}} \underline{\sigma} : \underline{\epsilon}(\overrightarrow{D})dv$. This last expression corresponds to the total potential energy theorem $\delta\mathscr{V} = \delta(\mathscr{U} -$

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[4]Virtual work and static equilibrium are two dual notions. More generally, virtual powers and dynamic equilibrium are two dual notions. If one is postulated as a principle, the other becomes a theorem.

$\mathscr{T}) = 0$ where $\mathscr{U}$ is the strain energy and $\mathscr{T}$ the work of external forces and volumetric forces[5]. There is a wealth of literature illustrating these examples.

Another possible pedagogical choice is to balance the forces at the nodes. Consider that forces act at the nodes to deform the elements. Conversely, the deformed elements induce forces on the nodes. These forces are called *generalized nodal forces*. In order to remain compatible with the laws of physics (energy conservation[6]), we will quantify these generalized forces so that the elastic deformation energy contained in the element corresponds to the work of the generalized force in the corresponding displacement of the node, as illustrated in Fig. 5. The element can be seen as an object
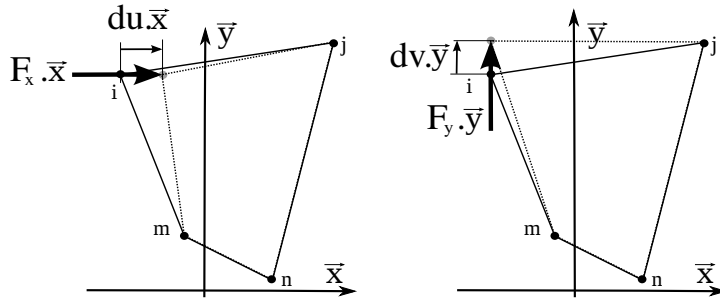

Figure 5: x-component of the generalized force at node i (left) and y-component (right).

whose edges must follow a shape imposed by the interpolation function. If a node is moved, the adjacent edges follow the movement as if they had

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[5]However, a particular point must be stressed: the stress field estimated by the finite element method is not always continuous from one element to another. Indeed, the displacements are continuous but through their derivatives. If the deformations present discontinuities at the passage from one element to another, then the stresses also present some. It is as if external forces corresponding to these discontinuities were acting at the boundaries of the elements. Let us recall that under the respect of SPH in linear elasticity, the solution is unique. If it respects the law of behaviour, equilibrium and boundary conditions everywhere, in other words if it is statically and kinematically admissible and respects the law of behaviour everywhere, then it is the only exact solution of the problem. In the case of the solution obtained by the finite element method, except for special cases of absence of these discontinuities (uniform fields for example which can be exactly described by the interpolation functions), the solution is not statically admissible due to discontinuities in the stress field at the boundaries of the elements and is therefore not exact. Nevertheless, it is kinematically admissible and respects the behaviour law. However, it can be considered accurate for the given problem to which we would add external forces corresponding to these discontinuities acting at the element boundaries. If these "parasitic" forces are made to work in the displacements of the element boundaries, we can then have a form of quantification of the error committed by comparing it to the deformation energy of the domain. Some software programs use this procedure to calculate an error indicator.

[6]Note that using the expression for the strain energy density in the form $\underline{\underline{\sigma}} : \underline{\underline{\epsilon}}$ implies the energy balance of the volume element.

rigidity and one can imagine that a point force is acting at the node. For example in any deformation state, if only one change du_i is non-zero then F_{xi} must be such that the deformation energy of the element, denoted by $E_{el.}$, increases by $dE_{el.} = F_{xi}du_i$ which corresponds to the work of F_{xi} in the small displacement du_i, i. e.:

$$F_{xi} = \frac{\partial}{\partial u_i} E_{el.} \tag{25}$$

For the moment, it is assumed that there is no external force applied to the node other than F_{xi} that deforms the element. Later, other forces can be superimposed. The elastic energy "contained" in the element is:

$$E_{el.} = \int\int_{element} \mathscr{E}_{el.}(x,y) \, dxdy \tag{26}$$

where $\mathscr{E}_{el.}$ denotes the elastic energy density which is given by $\mathscr{E}_{el.} = \frac{1}{2}(\epsilon_{xx}\sigma_{xx} + \epsilon_{yy}\sigma_{yy} + 2\epsilon_{xy}\sigma_{xy})$ or with the vector notation which is much more convenient for computer programming $\mathscr{E}_{el.} = \frac{1}{2}(\epsilon_1\sigma_1 + \epsilon_2\sigma_2 + \epsilon_3\sigma_3)$.

$$2\mathscr{E}_{el.} = [\epsilon_1\epsilon_2\epsilon_3]\begin{bmatrix}\sigma_1\\\sigma_2\\\sigma_3\end{bmatrix} = [\epsilon_1\epsilon_2\epsilon_3]\mathbf{C}\begin{bmatrix}\epsilon_1\\\epsilon_2\\\epsilon_3\end{bmatrix} = (\mathbf{qB})^T\mathbf{CBq} = \mathbf{q}^T\mathbf{B}^T\mathbf{CBq} \tag{27}$$

Recall that $\mathbf{q} = [u_i, u_j, u_m, u_n, v_i, v_j, v_m, v_n] = [q_1, q_2, q_3, q_4, q_5, q_6, q_7, q_8]$ is the vector of nodal unknowns related to the element for the instant considered.

$$F_i = \frac{\partial}{\partial q_i}\int\int_{element}\frac{1}{2}\mathbf{q}^T\mathbf{B}^T\mathbf{CBq} = \frac{1}{2}\frac{\partial}{\partial q_i}\mathbf{q}^T[\int\int_{element}\mathbf{B}^T\mathbf{CB}]\mathbf{q} \tag{28}$$

the volume integration only concerns the term $textbf{B}^T\mathbf{CB}$ since it alone depends on (x,y) (or (a,b) according to the space considered, real or parametric). The term $textbf{K} = \int\int_{element}\mathbf{B}^T\mathbf{C}$ is called the stiffness matrix of the element. The volume integration technique in the element will be explained later. The result is:

$$F_i = \frac{\partial}{\partial q_i}\frac{1}{2}\sum_{i=1}^{8}\sum_{j=1}^{8}q_iK_{ij}q_j = \sum_{j=1}^{8}K_{ij}q_j$$

Hence, by designating $[F_{xi}, F_{xj}, F_{xm}, F_{xn}, F_{yi}, F_{yj}, F_{yn}, F_{ym}]$ par $[F_1, F_2, F_3, F_4, F_5, F_6, F_7, F_8]$:

$$\mathbf{F} = \begin{bmatrix}F_1\\F_2\\F_3\\F_4\\F_5\\F_6\\F_7\\F_8\end{bmatrix} = \mathbf{K}\begin{bmatrix}q_1\\q_2\\q_3\\q_4\\q_5\\q_6\\q_7\\q_8\end{bmatrix} = \mathbf{Kq} \tag{29}$$

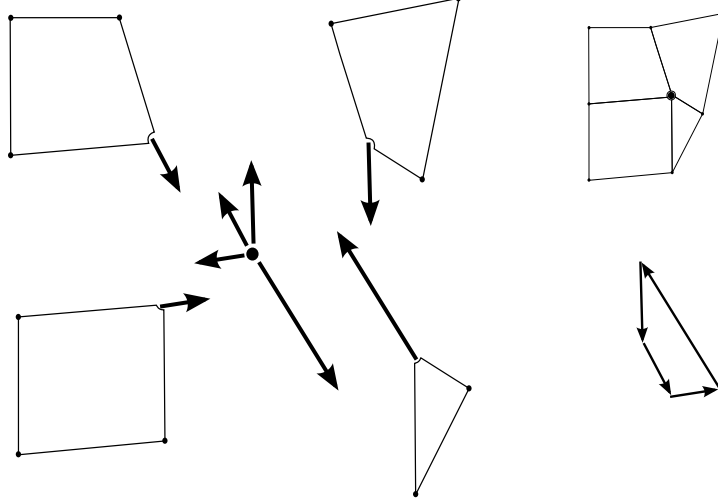As shown in Fig. 6, it will then be necessary to consider that the forces

Figure 6: Balance of forces generalized to a node. The actions of the node on the elements are opposite to the reactions of the elements on the node. The sum of the force vectors must give the zero vector.

generalised to the nodes are balanced, i.e. that the sum of the components according to $\overrightarrow{x}$ is zero as well as the sum of the components according to $\overrightarrow{y}$. There will therefore be 2 equations per node and we note that there are two unknowns, u_i and v_i, per node in general in solid mechanics, inside the domain the unknowns are the nodal displacements, at the boundary it is possible that the unknown is a reaction force. The result is a system of N equations with N unknowns where N = 2 times the number of nodes in our example. We must now calculate the integral of equation 26 which is the same as that of equation 28.

3.8. Volume integration

The example chosen to illustrate this course is in two dimensions. We will therefore consider for the volume integration a unit of thickness $z_{th.} = 1$. The surface ds of Fig. 7 in real space corresponds to the surface $ds' = dadb$ in parametric space where $\overrightarrow{a} \perp \overrightarrow{b}$. Let us note $\overrightarrow{d\mathscr{A}}$ the path travelled in real space (x, y) when $da\overrightarrow{a}$ is travelled in parametric space and respectively $\overrightarrow{d\mathscr{B}}$ for $db\overrightarrow{b}$. These vectors are expressed as $\overrightarrow{d\mathscr{A}} = (\frac{\partial x}{\partial a}\overrightarrow{x} + \frac{\partial y}{\partial a}\overrightarrow{y})da$ and $\overrightarrow{d\mathscr{B}} = (\frac{partialx}{partialb}\overrightarrow{x} + \frac{\partial y}{\partial b}\overrightarrow{y})db$. As the vectors $\overrightarrow{d\mathscr{A}}$ and $\overrightarrow{d\mathscr{B}}$ may not be perpendicular, the area must be calculated from the vector product:

$$dv_{real} = z_{th.}ds = z_{th.}(\overrightarrow{d\mathscr{A}} \wedge \overrightarrow{d\mathscr{B}}) = z_{th.}\begin{bmatrix} J_{11}da \\ J_{12}da \end{bmatrix} \wedge \begin{bmatrix} J_{21}db \\ J_{22}db \end{bmatrix}$$

which gives $dv_{real} = z_{th.}(J_{11}J_{22} - J_{12}J_{11})dadb = det.(\mathbf{J})dadb$ where $det.(\mathbf{J})$ is of course calculated at the point with coordinates (a, b). It may be possible
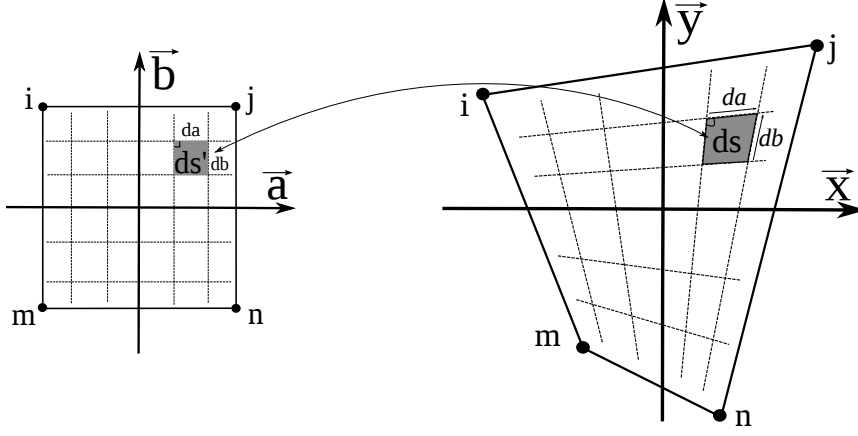
Figure 7: Transformation of a surface element from parametric space (left) to real space (right).

to write $det.(\mathbf{J})_{(a,b)}$ to make it easier to remember. The change of variables in equation 26 to go from (x, y) to (a, b) thus gives for the volume integration in two dimensions and a thickness $z_{th.}$:

$$\mathscr{I} = z_{th.} \int \int_{element} \mathscr{E}(x, y) \; dxdy = z_{th.} \int_{-1}^{+1} \int_{-1}^{+1} e(a, b) \; det.(\mathbf{J}) \; dadb$$

where $\mathscr{E}(x, y)$ denotes a density or a weighting, which depends on the nature of the problem treated, and $e(a(x, y), b(x, y))$ denotes the density or weighting corresponding to $\mathscr{E}(x(a, b), y(a, b))$, which is explicitly expressed from the nodal unknowns q_i and (a, b). Note that $det.(\mathbf{J})$ is also expressed explicitly from the nodal coordinates x_i and y_i and (a, b). The integral $\mathscr{I}$ can therefore be calculated. The method used to calculate this integral numerically is classically the Gauss method (see for example [14] for more information). It consists in making a weighted sum of n_G values $e(a, b)det.(\mathbf{J}_{(a,b)})$ to arrive at:

$$\mathscr{I} \approx z_{th.} \sum_{i=1}^{n_G} w_i \; e(a, b) \; det.(\mathbf{J})_{(a,b)} \qquad (30)$$

Although the Gaussian method can provide an exact value for polynomials, the result is usually not an exact value but still suitable. In our case, if we use four points for the Gaussian integration, i. e. $n_G = 4$, the weights are 1, i. e. $w_i = 1, \forall i$ and the integral becomes:

$$\mathscr{I} \approx z_{th.}\{e(\frac{-1}{\sqrt{3}}, \frac{-1}{\sqrt{3}}) \; det.(\mathbf{J})_{(\frac{-1}{\sqrt{3}}, \frac{-1}{\sqrt{3}})} + e(\frac{1}{\sqrt{3}}, \frac{-1}{\sqrt{3}}) \; det.(\mathbf{J})_{(\frac{1}{\sqrt{3}}, \frac{-1}{\sqrt{3}})}$$

$$+ e(\frac{-1}{\sqrt{3}}, \frac{1}{\sqrt{3}}) \; det.(\mathbf{J})_{(\frac{-1}{\sqrt{3}}, \frac{1}{\sqrt{3}})} + e(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}) \; det.(\mathbf{J})_{(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}})}\}$$

3.9. Assembly

Assembly is the term commonly used for the operation which consists of obtaining the stiffness matrix of the whole structure. It consists of assembling the elementary stiffness matrices. Consider a node i that belongs to elements C and E. It is possible that a given external force, denoted by $\overrightarrow{F_i^{ext.}}$ is applied to this node. The action of element E on node i, $-\overrightarrow{F_i^E}$, corresponds to the reaction of node i on element E denoted by $\overrightarrow{F_i^E}$. This force is given by equation 29 which must be completed, here with an exponent ^{E} or ^{C}, to specify the element considered. So we write $F^E = K^E q^E$ for the element E and $F^C = K^C q^C$ for the element C. If only the elements C and E are linked to node i, it comes:

$$\begin{bmatrix} F_x^C \\ F_y^C \end{bmatrix} + \begin{bmatrix} F_x^E \\ F_y^E \end{bmatrix} - \begin{bmatrix} F_x^{ext.} \\ F_y^{ext.} \end{bmatrix} = 0 \tag{31}$$

This equation expresses the equilibrium of node i which belongs to elements C and E. The equilibrium of the structure will be formalised by expressing the equilibrium of all the nodes. Let us denote by **d** the vector which contains all the nodal displacements and by **f** the vector which contains all the external nodal forces. If the structure has N_N nodes and N_E elements, then the equilibrium of the structure can be expressed by:

$$f_g = \sum_{k=1}^{N_N} (\sum_{m=1}^{N_E} K_{gk}^m) d_k = \sum_{k=1}^{N_N} \mathbb{K}_{gk} d_k \tag{32}$$

If element n does not contain both g and k nodes, then $K_{gk}^n = 0$. There is therefore generally a very high proportion of zero values in the stiffness matrix of the structure. Furthermore, let us return to equ. 27 and consider the term in the ith row and j^{th} column of $\mathbf{B}^T \mathbf{C} \mathbf{B}$:

$$[B^T C B]_{ij} = \sum_k \sum_l [B^T]_{ik} [C]_{kl} [B]_{lj}$$
$$= \sum_k \sum_l [B]_{ki} [C]_{kl} [B]_{lj} = \sum_k \sum_l [B]_{ki} [C]_{kl} [B^T]_{jl}$$

since $[C]_{kl} = [C]_{lk}$ we can rearrange the terms to obtain:

$$[B^T C B]_{ij} = \sum_k \sum_l [B^T]_{jl} [C]_{lk} [B]_{ki} = [B^T C B]_{ji}$$

which shows that $\mathbb{K}$ is symmetric. Techniques for storing and inverting such matrices, which are symmetric with many zero values, have therefore been developed. The system finally obtained is written $\mathbb{K}\mathbf{d} = \mathbf{f}$

3.10. Border conditions and resolution

Considering a node i and a direction, for example $\overrightarrow{x}$, there are two possibilities to express its condition:
- the displacement u_i along $\overrightarrow{x}$ is known. The force f_i along $\overrightarrow{x}$ is then a

priori unknown,

- lhe force f_i along $\overrightarrow{x}$ is known. The displacement u_i along $\overrightarrow{x}$ is then a priori unknown.

The directions $\overrightarrow{x}$ and $\overrightarrow{y}$ are independent of these conditions so that we can know the displacement along $\overrightarrow{x}$ and the force along $\overrightarrow{y}$. The external force can be zero. In the example of Fig. 8 the boundary conditions are:

- all displacements are unknown except for $u_s = v_s = u_l = v_l = u_p = v_p = 0$ and $v_i = 0$,

- all sums of nodal forces are known and zero ($F_{xm} = 0, F_{ym} = 0, F_{xi} = 0,$ ...) except $F_{yk} = P_1, F_{xo} = P_2$ and $F_{yo} = P_3$ which are non-zero and $F_{yi}, F_{xs}, F_{ys}, F_{xl}, F_{yl}, F_{xp}, F_{yl}$ are unknown support reactions which will be determined by the resolution.

For this example with 11 nodes, we end up with a system of 22 equations with 22 unknowns. For a system of minimal size ($22 \otimes 22$), it is then necessary to group the unknown terms in a vector and the known terms in another one then to constitute the matrix corresponding to the system to be solved. Two other classical methods exist to constitute the system, the method by *penalisation* and the method of *Lagrange multipliers.*

- The method by penalisation provides a result close to the solution but can pose problems of matrix conditioning. Not detailed here, it is explained in numerous works such as [19].

- The method of Lagrange multipliers consists in increasing the system. For our example the system to be solved would be of size $((22 + 7) \otimes (22 + 7))$ because there are 7 displacements imposed so 7 additional equations and 7 corresponding support reactions which become 7 additional unknowns. By this method, although the size of the system increases, the computer processing is simpler and the result of the numerical inversion remains exact [19] [14].
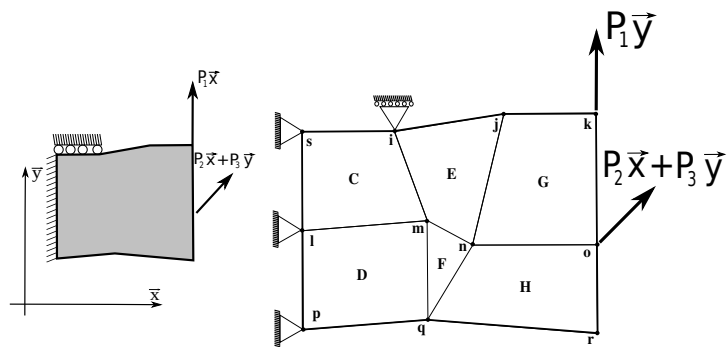

Figure 8: Example of modelling boundary conditions.

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3.11. Finite element softwares

It is necessary to find a compromise between simplicity of use and the possibility of solving, or even customising, the problem. Among the free software, we can mention the excellent ASTER and SATURNE codes developed by EDF, which can be found at http://www.code-aster.org (preferably for solid mechanics) and http://code-saturne.org (preferably for fluid mechanics). However, their handling and installation is not the easiest. Not free but graciously given to academics with its sources, a little easier to handle, we can quote the CAST3M code. The latter is used for the examples of this course, it can be found at http://www-cast3m.cea.fr.

4. Finite difference method

4.0.1. Taylor's expansion

The finite difference method consists in differentiating between the noeuds. Only the principle is explained here. Let us take the example of a calculation of heat diffusion in the (x, y) plane, the temperature being $T(x, y)$. Recall that the Taylor series expansion allows us to write:

$$T(x + dx, y) = T(x, y) + \frac{dx}{1!}\frac{\partial T}{\partial x}\Big|_{|(x,y)} + \frac{dx^2}{2!}\frac{\partial^2 T}{\partial x^2}\Big|_{(x,y)} + \frac{dx^3}{3!}\frac{\partial^3 T}{\partial x^3}\Big|_{(x,y)} + ...$$

$$T(x - dx, y) = T(x, y) - \frac{dx}{1!}\frac{\partial T}{\partial x}\Big|_{|(x,y)} + \frac{dx^2}{2!}\frac{\partial^2 T}{\partial x^2}\Big|_{(x,y)} - \frac{dx^3}{3!}\frac{\partial^3 T}{\partial x^3}\Big|_{(x,y)} + ...$$

The first derivative can therefore be obtained from:

$$T(x + dx, y) - T(x - dx, y) = \frac{2dx}{1!}\frac{\partial T}{\partial x}\Big|_{|(x,y)} + \frac{2dx^3}{3!}\frac{\partial^3 T}{\partial x^3}\Big|_{(x,y)} + ...$$

since $dx^3 << dx$, it comes:

$$\frac{\partial T}{\partial x}\Big|_{(x,y)} \approx \frac{T(x + dx, y) - T(x - dx, y)}{2dx}$$

The second derivative can therefore be obtained from:

$$T(x + dx, y) + T(x - dx, y) = 2T(x, y) + \frac{2dx^2}{2!}\frac{\partial^2 T}{\partial x^2}\Big|_{(x,y)} + \frac{2dx^4}{4!}\frac{\partial^4 T}{\partial x^4}\Big|_{(x,y)} ...$$

since $dx^4 << dx^2$, it comes:

$$\frac{\partial^2 T}{\partial x^2}\Big|_{(x,y)} \approx \frac{T(x + dx, y) + T(x - dx, y) - 2T(x, y)}{dx^2}$$

4.0.2. Calculation of the gradient

In practice dx is not very small but corresponds to the distance Δx between two lines of neighboring nodes. Let us consider the mesh of Fig. 9.
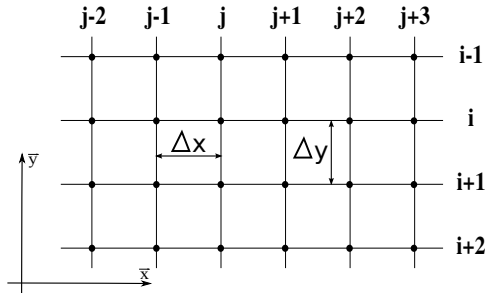
Figure 9: Example of a mesh used in finite difference.

For the sake of simplicity in the presentation of the principle of the method, this one is considered square, i.e. $\Delta x = \Delta y$, we obtain:

$$\frac{\partial T}{\partial x}_{|(x,y)} \approx \frac{T(x + \Delta x, y) - T(x - \Delta x, y)}{2\Delta x} = \frac{T_{j+1} - T_{j-1}}{2\Delta x} \qquad (33)$$

where we can replace Δx by Δy and j by i to differentiate according to y.

4.0.3. Calculation of the Laplacian

$$\frac{\partial^2 T}{\partial x^2}_{|(x,y)} \approx \frac{T(x + \Delta x, y) + T(x - \Delta x, y) - 2T(x,y)}{\Delta x^2} = \frac{T_{j+1} + T_{j-1} - 2T_j}{\Delta x^2}$$
$$(34)$$

where we can replace Δx by Δy and j by i to differentiate according to y. One of the drawbacks of the method is the need for a regular mesh or a geometric transformation of this regular mesh.

4.0.4. On-board conditions and resolution

For a steady state heat diffusion calculation the edge conditions must be expressed. At a node, either the temperature is imposed or the flux is imposed. It is of course necessary to make some assumptions in order to extend the calculated evolutions on one side for the nodes which have no neighbor on the other side. This is another drawback of the method.

5. Finite volume method

In the finite volume method, the integrals of a conservation or equilibrium law, i. e. divergence terms, are transformed into surface integrals using the flux-divergence theorems. Instead of expressing conservation or equilibrium at a point (at the node), we express it for a finite volume. In heat conduction and in the steady state, for example, we express that *flow into the volume = flow out of the volume* instead of writing $\triangle T = 0$. This formulation can sometimes be more robust than the finite element formulation because it avoids a derivation.
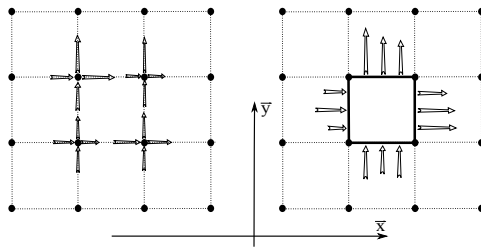
Figure 10: Finite volume calculation principle. On the left the classical formulation at the nodes. On the right the finite volume formulation. The arrows symbolize for example incoming and outgoing heat flows.

6. Boundary element method

6.1. General information about the boundary element method

The boundary element method allows to solve many problems for which the discretization of a volume is a problem. Indeed, with this method, only the surface requires discretization. It is commonly used in acoustics, solid mechanics, aerodynamics, electromagnetism, diffusion, etc. The boundary elements method can be the subject of a lengthy course, but in summary it is important to know that:

- Only the domain boundary needs to be discretized. It is composed of distinct elements. The fields are interpolated inside the elements from the nodal values.

- It is based on Green's functions and therefore assumes a linear behavior, a homogeneous medium and the possibility to superimpose these exact analytical solutions.

- It consists in superimposing at best[7] distributions at the boundaries (in solid mechanics, for example, they are distributions of forces or displacements on boundary elements) to obtain a solution in the domain concerned[8].

- The solution is better in the domain far from the boundaries because the fields are less sensitive to the imperfections of the respect of the boundary conditions by the interpolation functions of the elements.

- The points where the field values must be computed must be specified during the post-processing of the solution.

- If the behavior is non-linear, it is possible to use solutions based on Green's functions, but the interest of the method is lost because the part of the domain in which there are non-linearities must be discretized. One distributes there fictitious volume actions leading to the same effects as those of the

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[7]The quality depends on the appropriateness of the shape of the chosen distributions.

[8]Green's solutions are valid in infinite or semi-infinite media, only values for the points located inside the domain have a physical meaning and are calculated.

nonlinearities of behavior[9]. As always, in this case one must proceed by iterations.

- The matrix obtained is not symmetrical and one cannot use the algorithms developed for the finite elements. Nevertheless, it should be noted that the size of the system is much smaller than with the finite element method since we go down one dimension of space by passing from the volume to its surface.

6.2. The boundary element method applied to isotropic linear elasticity

In linear elasticity, we can use the reciprocity theorem, also called Somigliana identity:

$$\int_{\mathscr{D}} \underline{\underline{\sigma}} : \underline{\underline{\epsilon}}^* \ dv = \int_{\mathscr{D}} \underline{\underline{\underline{C}}}.\underline{\underline{\epsilon}} : \underline{\underline{\epsilon}}^* \ dv = \int_{\mathscr{D}} \underline{\underline{\epsilon}} : \underline{\underline{\underline{C}}}.\underline{\underline{\epsilon}}^* \ dv = \int_{\mathscr{D}} \underline{\underline{\sigma}}^* : \underline{\underline{\epsilon}} \ dv$$

because the tensor of compliances $\underline{\underline{\underline{C}}}$ is symmetric. The virtual work theorem expresses that:

$$\int_{\mathscr{D}} \underline{\underline{\sigma}} : \underline{\underline{\epsilon}}(\overrightarrow{D^*}) \ dv = \int_{\partial\mathscr{D}} \overrightarrow{T}\overrightarrow{D^*} \ ds + \int_{\mathscr{D}} \overrightarrow{\mathfrak{g}}\overrightarrow{D^*} \ dv$$

where $\mathfrak{g}$ are volumetric forces. We can therefore deduce from these last two equations that:

$$\int_{\partial\mathscr{D}} \overrightarrow{T}\overrightarrow{D^*} \ ds + \int_{\mathscr{D}} \overrightarrow{\mathfrak{g}}\overrightarrow{D^*} \ dv = \int_{\partial\mathscr{D}} \overrightarrow{T^*}\overrightarrow{D} \ ds + \int_{\mathscr{D}} \overrightarrow{\mathfrak{g}^*}\overrightarrow{D} \ dv \qquad (35)$$

Now, to construct the boundary element method, the volume force $\overrightarrow{\mathfrak{g}^*}$ is chosen to be a unitary point force applied within an infinite medium whose solution was given by Kelvin as schematized in Fig. 11 at left. Let us consider that there is no volume force in the problem to be solved, i.e. $\overrightarrow{\mathfrak{g}} = \overrightarrow{0}$[10]. We
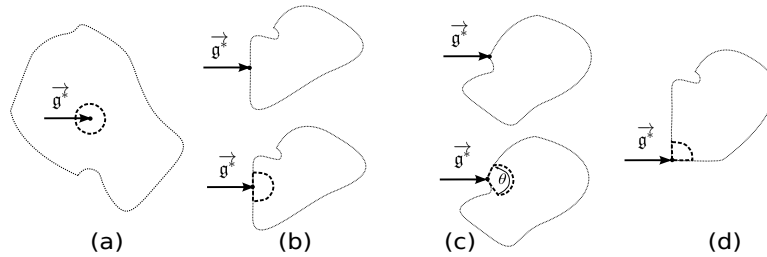

Figure 11: Unit point volume force applied to a point in the volume (left), to a point on a flat surface (middle), and to a corner point of an angular surface (right).

discretize the surface *partial*$\mathscr{D}$ into elements defined by nodes. If we apply

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[9]For example for an elastoplastic calculation in solid mechanics, one will superimpose fictitious volume forces which simulate the plastic deformation.

[10]Or else we have to integrate in the volume and we lose some interest in the method.

the unit force $\overrightarrow{\mathfrak{g}}$ to the node i of this surface for example in the direction $\overrightarrow{x}$, we can write:

$$\int_{\partial \mathscr{D}} \overrightarrow{T}\overrightarrow{D^*} \, ds = \int_{\partial \mathscr{D}} \overrightarrow{T^*}\overrightarrow{D} \, ds + \eta_i(\overrightarrow{U_i}.\overrightarrow{x}) \qquad (36)$$

where $\overrightarrow{U_i}$ is the displacement of the noeud i and η_i a coefficient which depends on the portion of volume integrated around i as schematized in Fig. 11. $\eta_i = 1$ if we integrate all around the point (Fig. 11a), $\eta_i = \frac{1}{2}$ if we integrate in a half-space around the point (Fig. 11b) and $\eta_i = f(\theta)$ if we integrate at an angular point of angle θ (Fig. 11c) for a two-dimensional problem (e.g. $f(\frac{\pi}{2}) = \frac{1}{4}$, Fig. 11d).

6.3. Spatial discretization and interpolation

Knowing the values at the nodes, we need to interpolate between the nodes in the same way as the finite element method. Let us assume for clarity, for our two-dimensional illustration, that the fields vary linearly by element. The element is a line segment bounded by two nodes. The force $\overrightarrow{\mathfrak{g}^*} = 1^* \overrightarrow{x}$, to denote a unit virtual force according to $\overrightarrow{x}$, is applied to node i. We can therefore write that:

$$\sum_{j=1}^{N} \int_{element \ j} \overrightarrow{T}\overrightarrow{D^*} \, ds = \sum_{j=1}^{N} \int_{element \ j} \overrightarrow{T^*}\overrightarrow{D} \, ds + \eta_i u_i$$

The element j is defined by the nodes m and n. The surface stress vector at node m is $\overrightarrow{T_m} = t_{xm}\overrightarrow{x} + t_{ym}\overrightarrow{y}$. The displacement vector of node m is $\overrightarrow{U_m} = u_m\overrightarrow{x} + v_m\overrightarrow{y}$. The constraint vector between m and n is interpolated and the component, according to $\overrightarrow{x}$, for example is $\alpha t_{xn} + (1-\alpha)t_{xm}$ in the element j if α varies from 0 to 1 going from m to n.

$$\sum_{j=1}^{N} \int_{element \ j} \overrightarrow{T}\overrightarrow{D^*} \, ds = \sum_{j=1}^{N} \int_{element \ j} \overrightarrow{T^*}\overrightarrow{D} \, ds + \eta_i u_i$$

Consider the first term of this equality. If L_j denotes the length of element j, using linear interpolation we get:

$$\int_{element \ j} \overrightarrow{T}\overrightarrow{D^*} \, ds =$$

$$\int_{\alpha=0}^{\alpha=1} [(\alpha t_{xn} + (1-\alpha)t_{xm})\overrightarrow{x} + (\alpha t_{yn} + (1-\alpha)t_{ym})\overrightarrow{y}]\overrightarrow{D^*}(\alpha) \ L_j d\alpha$$

where L_j plays the role of the determinant of the Jacobian matrix. The integration is usually done with classical numerical techniques. After integration, one will thus obtain expressions of the type, for a unit force $\overrightarrow{\mathfrak{g}^*}$ applied at i along $\overrightarrow{x}$:

$$\int_{element \ j} \overrightarrow{T}\overrightarrow{D^*} \, ds = g_{xijxm}t_{xm} + g_{xijxn}t_{xn} + g_{xijym}t_{ixym} + g_{xijyn}t_{ixyn}$$

$$\int_{element\ k} \overrightarrow{T}\overrightarrow{D^*}\,ds = g_{xikxn}t_{xn} + g_{xikxp}t_{xp} + g_{xikyp}t_{yp} + g_{xikypn}t_{yp}$$

6.4. Construction of a linear system of equations

After summation and factorization we get coefficient terms of the nodal values $G_{xixn} = \sum_{j=1}^{N} g_{xijxn}$. The term G_{xixn} relates to a unit force $\overrightarrow{\mathfrak{g}^*}$ applied at node i along $\overrightarrow{x}$ and the component along $\overrightarrow{x}$ of the force $\overrightarrow{T}$ at node n. In the same way, we can make terms of type H_{xixn} appear. The latter, H_{xixn}, concerns a unit force $\overrightarrow{\mathfrak{g}^*}$ applied to node i along $\overrightarrow{x}$ and the component along $\overrightarrow{x}$ of the displacement $\overrightarrow{U}$ of node n. We finally obtain two
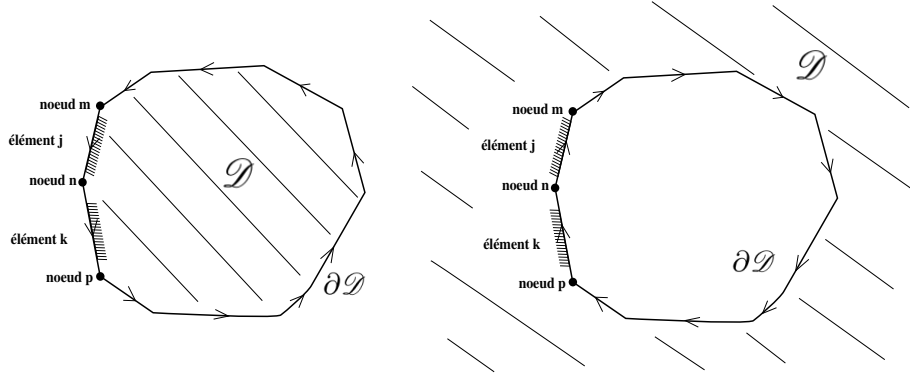

Figure 12: Domain, domain boundary, nodes and oriented elements - for example matter is always on the left in positive progression. Finite medium on the left and hole in an infinite medium on the right.

equations for each node i:

$$G_{xixn}t_{xn} + G_{xiyn}t_{yn} = H_{xixn}u_n + H_{xiyn}v_n + \eta_i u_i$$

$$G_{yixn}t_{xn} + G_{yiyn}t_{yn} = H_{yixn}u_n + H_{yiyn}v_n + \eta_i v_i \tag{37}$$

At each node i, we know either t_{xi} or u_i for the component along $\overrightarrow{x}$ and either t_{yi} or v_i for the component along $\overrightarrow{y}$. This allows to group the unknown terms on one side of the equality to obtain a linear system of equations.

6.5. Calculation of coefficients η_i

The coefficients η_i are simply computed by assuming a uniform rigid solid translation on the domain, for example $\overrightarrow{U} = \overrightarrow{x}\ \forall i$. From eq. 37 it follows:

$$\eta_i u_i = -H_{xixn}u_n - H_{xiyn}v_n + \zeta$$

$$0 = H_{yixn}u_n + H_{yiyn}v_n \tag{38}$$

where $\zeta = 0$ in finite medium and $\zeta = -\int_{\partial\mathscr{D}\infty} \overrightarrow{T^*}ds = 1$ in infinite medium.

There are few free software for computation with the boundary element method. However, one can find at www.bempp.org the excellent free code BEM++ which covers various problems of mechanics and physics in continuous media[11]. The sources of a code in Fortran for a program dedicated to plane elasticity are given in [6].

7. So-called "semi-analytical" methods

Semi-analytical (S. A.) methods consist in using analytical solutions for particular objects such as cracks, cavities, inclusions, heat sources, etc. As with the boundary element method, these solutions are superimposed as best as possible to satisfy the conditions of the problem. Contrary to the finite element or boundary element methods, they generally do not require any discretization of the medium, the geometry is defined by the position of the objects in space. Most of the time, they can naturally solve problems in infinite media. They can also be used to treat problems with singularities relatively easily. They are very powerful (good accuracy for a relatively small number of unknowns) for the expected objects but can only solve the types of problems involving these objects. In general, this type of method is used to make a large number of objects interact. Problems with singulari-
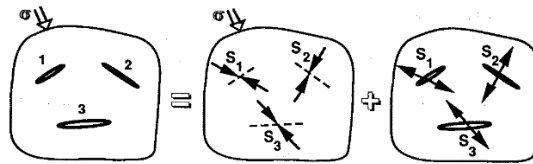

Figure 13: Some "objects" crack in a field applied at infinity. The problem to be solved becomes that of the interaction of the objects in the figure on the right.

ties require precautions regarding the interpolation functions in the vicinity of the singularities if one uses for example the finite element method (see Appendix C) or the boundary method. A semi-analytical method may be more appropriate in some cases, especially when the singularities are numerous. Let's take the example of the pseudo-traction method applied to cracks. The lips of a crack are free of normal and tangential stresses. If a cracked medium, which can be considered of infinite size compared to the size of the cracks, is subjected to a mechanical stress, for example a uniform tension at infinity, each crack acts as a perturbation of this tensile stress

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[11]Continuous and homogeneous media for this method. Nevertheless, one can solve problems in heterogeneous media but it will be necessary to assemble sub-problems in homogeneous media and to connect the boundary conditions appropriately.

field. We know the analytical solution for a crack in an infinite medium subjected to this type of loading. This solution is obtained considering that the crack is subjected to an internal pressure that cancels the tensile stress on its lips (Fig. 13 right). We therefore also know the stresses it induces at the location of another crack. If it induces an additional traction, then it will be necessary to apply an additional pressure in this other crack to cancel the stresses on its lips. The solution obtained will not be exact since the induced stress is not uniform (it decreases when moving away from the crack "object") and a uniform pressure will not be able to cancel it everywhere. We will therefore try to do the best we can - cancel the average of the stresses for example - to make the stress on the lips of this other crack minimal. As these cracks interact with each other and reciprocally, it will be necessary to write the unknown pressure problem in each crack properly. We can improve the accuracy, obviously at the expense of the number of unknowns (we go from one unknown per crack to two unknowns per crack), by using the analytical solution of a crack loaded by a linearly varying pressure. We can further improve the accuracy since we know the solutions for pressures that vary according to Legendre polynomial distributions. Obviously, the polynomial series must be limited to a finite number of terms. The method is detailed in [10]. It is an example of the use of Galerkin's method. A program with instructions and examples can be downloaded at http://site2christophe.chez.com/. The equivalent inclusion method is an-
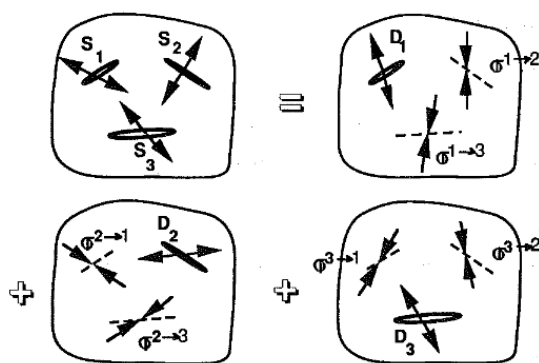

Figure 14: Superposition of the field perturbations related to the crack "objects". The problem is to determine the coefficients D_i in order to find the actions S_i as well as possible. The interaction matrix consists of the terms $\sigma^{i \rightarrow j}$.

other example of a semi-analytical method based this time on Taylor series. As proposed in [17], it is part of the collocation methods. It is important to note that it is not shown to converge. It even seems that it does not converge, which does not prevent it from providing satisfactory results in some cases. An alternative based on the minimization of the energy related to the normal and tangential stress discontinuities at the interfaces of the inclu-

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sions is proposed in [9] and should give better results. Thus reformulated, it is in line with the Ritz-Galerkin type methods.

8. Non-linear computations

Non-linear calculations are generally based on a linearization of the behavior by time increment. The temporal evolution is followed by updating the behavior and possibly the boundary conditions and geometry. There are two main classes of non-linear calculation schemes - The so-called "explicit" scheme which consists in progressing slowly with a large number of small increments. The parameters are updated at the end of each increment. - the so-called *implicit* scheme which consists in progressing by increments but which allows a return to the beginning of the increment to check the quality of the prediction. The updated parameters that allowed the prediction of the next solution must actually correspond to the next solution. For the same increment, the calculation is done in a loop until the difference between the estimated parameters and the updated parameters is smaller than a given standard. We refer to specialized books to deepen these notions: [20] [8] [15].

9. Example

The problem of the plate with holes in uniaxial tension is treated by three methods to illustrate advantages and disadvantages. The material is a steel of Young's modulus $E = 210\ GPa$ and Poisson's ratio $\nu = 0.33$. The calculation is conducted in plane stresses (P. Stre.), i. e. $\sigma_{zz} = 0$ for one unit of thickness. The plate is square of width $4\ a.u.$ and the hole of radius $1\ a.u.$ where "a.u." denotes an arbitrary unit of length. It is subjected to a uniaxial stress of axis y of $100\ MPa$ on the edges of type D-C, the other edges are free of stress as shown in Fig. 15. The spatial discretization is voluntarily coarse in order to show the imperfections of the methods. Indeed, very accurate results can be obtained with the tested methods when they are used with know-how and with computers of suitable power. The unknowns for the linked systems are:
- for the semi-analytical method (SA) of pseudo-tractions : at order 4, 5 unknowns per straight element and 10 unknowns per circular cavity. As the software does not allow for symmetry, the contour is discretized into 32 elements, which leads to $N = 1 * 10 + 5 * 32 = 170$ unknowns.
- for the boundary element method (BEM) : the problem takes into account the two symmetries. There are 29 nodes and two unknowns per node which leads to $N = 29 * 2 = 58$ unknowns. For the complete problem, a number of unknowns roughly equivalent to that of the S.A. method would be necessary.
- for the finite element method (FEM): the problem takes into account the two symmetries. There are 70 nodes and two unknowns per node which
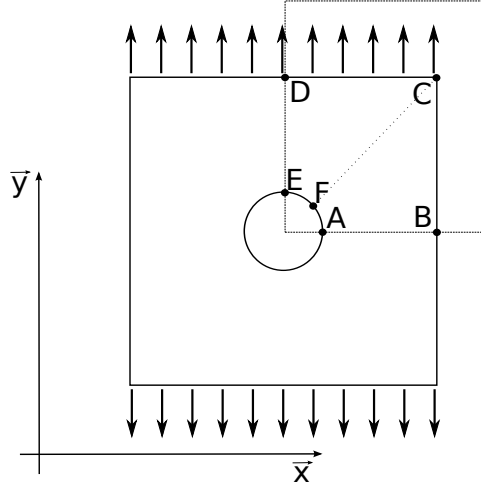
Figure 15: Plate with holes in uniaxial tension. The problem has two axes of symmetry.

leads to $N = 70 * 2 = 140$ unknowns. The knots of the contour are located at the same places as for the BEM method.

Aith a fine spatial discretization, the finite element method estimates the displacements u_y^E at point E at $1.725 \ 10^{-3}$ in P. Stre. and the stress concentration at point A at 359.4 MPa. The table 2 allows a comparison of the accuracies of the three different methods for a coarse discretization.

Methode	u_y^E (a.u.) P. Stre.	u_y^D (a.u.) P. Stre.	σ_{yy}^A (MPa) P. Stre.
SA	$1.728 \ 10^{-3}$	$2.62 \ 10^{-3}$	356.8
BEM	$1.703 \ 10^{-3}$	$2.60 \ 10^{-3}$	316.6
FEM	$1.651 \ 10^{-3}$	$2.58 \ 10^{-3}$	353.6

Table 2: Displacement along y of points E and D in P. Stre. and stress concentration in A.

The Figs. 17 present the evolution of stresses along profiles. σ_h and σ_{vm} respectively designate the hydrostatic and von Mises stresses[12].

We note that near the boundaries the boundary conditions are more difficult to respect by the BEM and SA methods, in particular in the corners of the plate. This is due to the singularities present in the basis functions used[13]. The BEM method presents strong inaccuracies near the boundaries,

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[12]$\sigma_{vm} = \sqrt{[(\sigma_{xx} - \sigma_{yy})^2 + (\sigma_{xx} - \sigma_{zz})^2 + (\sigma_{zz} - \sigma_{yy})^2]/2 + 3[\sigma_{xy}^2 + \sigma_{xz}^2 + \sigma_{zy}^2]}$

[13]These basis solutions (green functions, Boussinesq solution, etc.) are superimposed to obtain the best possible solution.
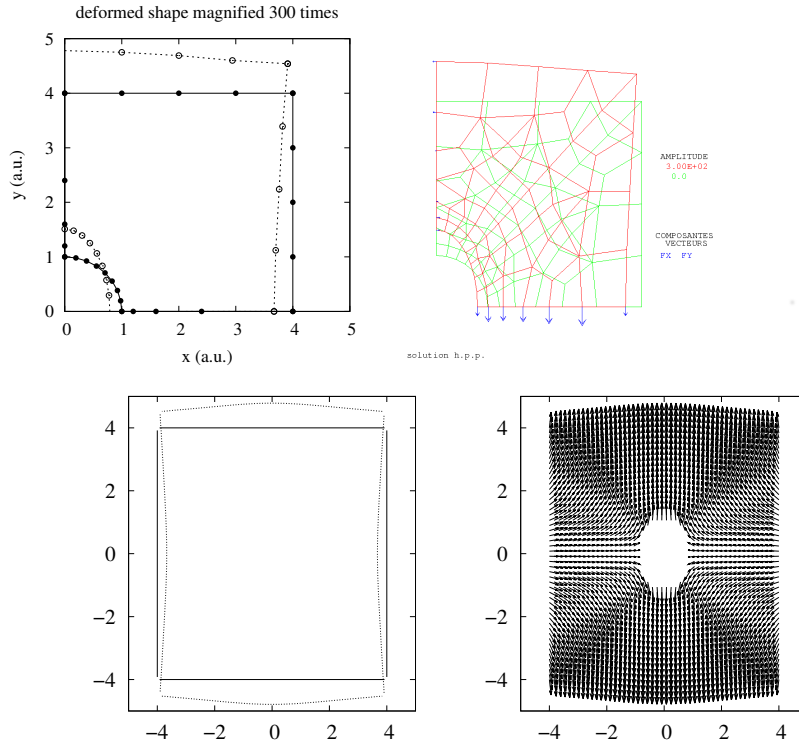
Figure 16: Spatial discretization and deformed shape for the boundary element method (top left) and for the finite element method (top right) and deformed and displacement vectors for the semi-analytical method (bottom).

especially since these boundaries are angular, at distances from the edge typically less than the length of the neighboring elements. As expected, the stress concentrations are well estimated by the SA method, but it should be noted that this method only treats this type of geometry (circular cavities for porosity[14]), unlike the other methods which can treat any cavity shape. The FEM method presents suitable results without any major drawback except the volume meshing and a computational power superior to the two other methods with equivalent accuracy. Fig. 18 shows the stress discontinuitiesrelated to the deformation discontinuities. The displacements are continuous but not their derivatives as they pass from one element to another. We recall that this is related to the interpolation functions whose domain of definition is limited to the element. Fig. 19 shows the isovals of the σ_{yy} stress obtained by BEM and SA. We notice that the edges are "heckled" by the BEM method. We also notice that the solution can be extended in the cavity for the SA method although this has, a priori, no

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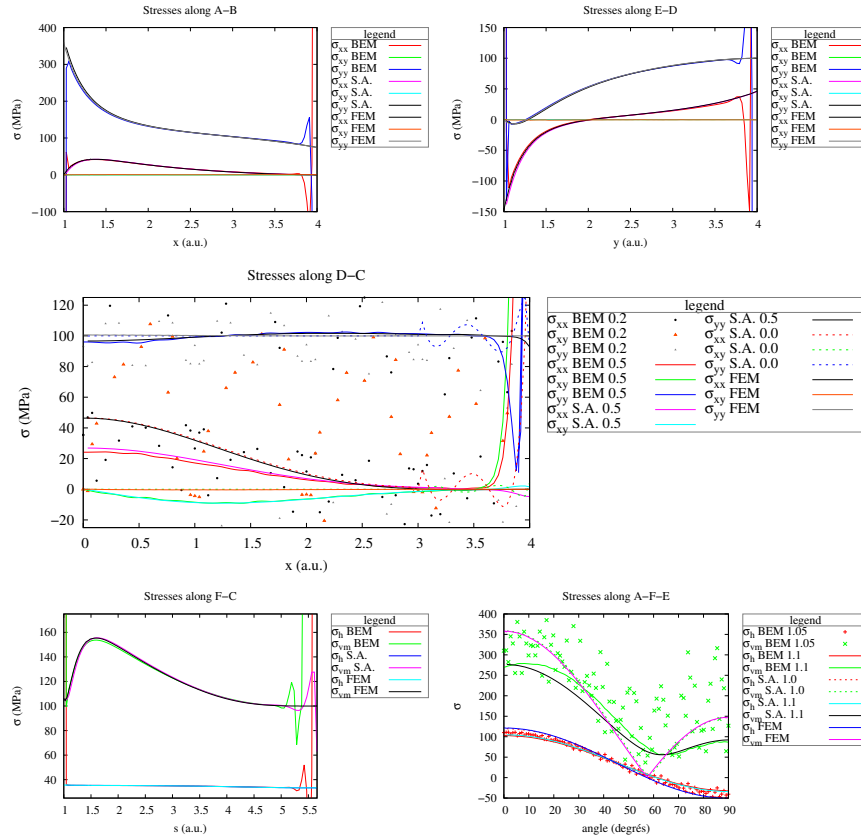[14]Non-intersecting straight cracks for damage.

Figure 17: Stress distributions along boundaries and for an F-C section. When a value is shown in the legend, it indicates how far from the boundary or on which radius the point where the stresses are calculated is located.

physical meaning. For the SA method, the constraint at point C is very poorly estimated because it is a corner[15]. On the other hand, it is very well estimated at point A with this method unlike the BEM. In conclusion, the BEM and FEM are more flexible than the SA method, which is only efficient for one type of problem. The FEM method appears to be the most robust. If there is no problem of spatial discretization or computational means, a "fine mesh" will provide excellent results. Moreover, the FEM method allows much more naturally than the two other methods to consider non-linear behaviors. It is therefore understandable why this method is the most widely developed and used.

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[15]With such methods, in this type of corner we have locally $sigma_{xy} \neq \sigma_{yx}$. The solution is not rigorously statically admissible... as for the FEM !
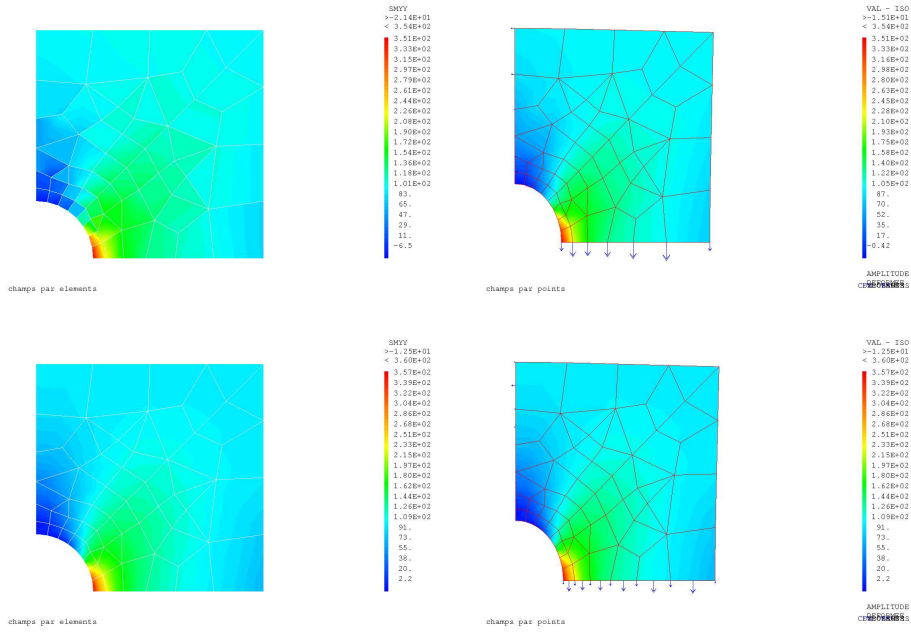
Figure 18: Map of the stress isovals σ_{yy} obtained by FEM. On the left the field per element, the real result of the calculation, which presents discontinuities and on the right the field per point which averages the values at the nodes for a more physical representation. On the top the calculation uses quadrilaterals with four nodes, on the bottom the calculation uses quadrilaterals with 8 nodes. The contour of the elements is the same in all cases.
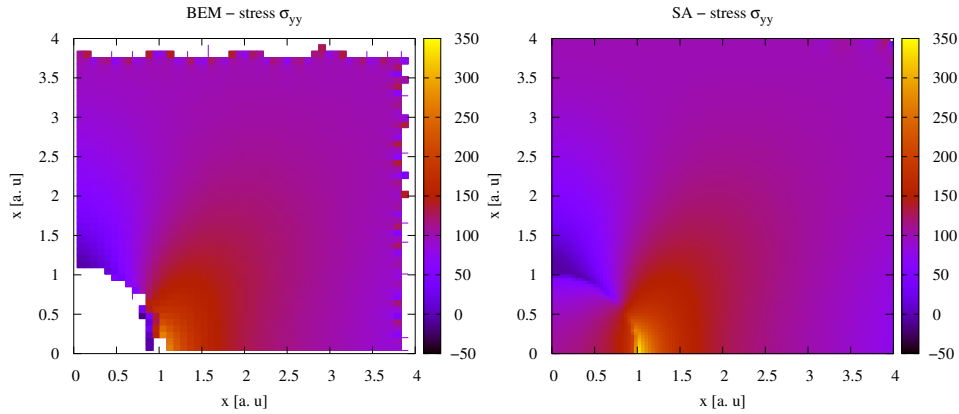

Figure 19: Map of σ_{yy} stress isovals obtained by BEM on the left and SA on the right.

Appendix A. Vector operators

The use of vector operators in the formalization makes it possible to get rid of the chosen coordinate system. Indeed, although the operators

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make the formulas less readable when one is not used to them, it is quite convenient that the equations thus formalized remain the same in Cartesian, cylindrical and spherical coordinates. The symbolic correspondences are given here for a Cartesian coordinate system with an example of a cylindrical coordinate system for the gradient operator. For another coordinate system, please refer to the equations corresponding to the operator used. Here are some of the commonly used operators:

$\overrightarrow{grad}$ designates the operator *"gradient"*. In a three dimensional Cartesian frame of reference it corresponds to $\overrightarrow{grad}(A) = \frac{\partial}{\partial x}(A)\overrightarrow{x} + \frac{\partial}{\partial y}(A)\overrightarrow{y} + \frac{\partial}{\partial z}(A)\overrightarrow{z}$. En cylindrical coordinates this operator becomes $\overrightarrow{grad}(A) = \frac{\partial}{\partial r}(A)\overrightarrow{r} + \frac{1}{r}\frac{\partial}{\partial \theta}(A)\overrightarrow{\theta} + \frac{\partial}{\partial z}(A)\overrightarrow{z}$. If $\overrightarrow{U}$ is a vector, then its gradient at the material point P is a tensor $\underline{\underline{grad}}(\overrightarrow{U})$ which is worth:

$$\underline{\underline{grad}}(\overrightarrow{U}) = \begin{bmatrix} \frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} & \frac{\partial u}{\partial z} \\ \frac{\partial v}{\partial x} & \frac{\partial v}{\partial y} & \frac{\partial v}{\partial z} \\ \frac{\partial w}{\partial x} & \frac{\partial w}{\partial y} & \frac{\partial w}{\partial z} \end{bmatrix}_P$$

in Cartesian coordinate system. In cylindrical coordinates this operator becomes:

$$\underline{\underline{grad}}(\overrightarrow{U}) = \begin{bmatrix} \frac{\partial u}{\partial r} & \frac{1}{r}\frac{\partial u}{\partial \theta} - \frac{v}{r} & \frac{\partial u}{\partial z} \\ \frac{\partial v}{\partial r} & \frac{1}{r}\frac{\partial v}{\partial \theta} + \frac{u}{r} & \frac{\partial v}{\partial z} \\ \frac{\partial w}{\partial r} & \frac{1}{r}\frac{\partial w}{\partial y} & \frac{\partial w}{\partial z} \end{bmatrix}_P$$

div designates the operator *"divergence"*. In a three dimensional Cartesian frame of reference it corresponds to $div(\overrightarrow{q}) = \frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z}$. Si $\underline{\underline{\sigma}}$ is a tensor, the operator provides:

$$\overrightarrow{div}(\underline{\underline{\sigma}}) = \begin{bmatrix} \frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} + \frac{\partial \sigma_{xz}}{\partial z} \\ \frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} + \frac{\partial \sigma_{yz}}{\partial z} \\ \frac{\partial \sigma_{xz}}{\partial x} + \frac{\partial \sigma_{yz}}{\partial y} + \frac{\partial \sigma_{zz}}{\partial z} \end{bmatrix}$$

$\triangle$ designates the operator *"laplacian"*. In a Cartesian frame of reference in three dimensions it corresponds to $\triangle = \frac{\partial^2}{\partial x^2}(\ ) + \frac{\partial^2}{\partial y^2}(\ ) + \frac{\partial^2}{\partial z^2}(\ )$

$\overrightarrow{\nabla}$ designates the operator *"Nabla"*. In a three dimensional Cartesian frame of reference it corresponds to $\overrightarrow{\nabla} = \frac{\partial}{\partial x}(\ )\overrightarrow{x} + \frac{\partial}{\partial y}(\ )\overrightarrow{y} + \frac{\partial}{\partial z}(\ )\overrightarrow{z}$. Let us note the correspondences of notations $\overrightarrow{\nabla}f = \overrightarrow{grad}f$ et $\overrightarrow{\nabla}.\overrightarrow{A} = div(\overrightarrow{A})$ and at the

spatial point P :

$$\nabla^2(\overrightarrow{V}) = \begin{bmatrix} \frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2} + \frac{\partial^2 v_x}{\partial z^2} \\ \frac{\partial^2 v_y}{\partial y^2} + \frac{\partial^2 v_y}{\partial y^2} + \frac{\partial^2 v_y}{\partial z^2} \\ \frac{\partial^2 v_z}{\partial x^2} + \frac{\partial^2 v_z}{\partial y^2} + \frac{\partial^2 v_z}{\partial z^2} \end{bmatrix}_P$$

The operator $Tr()$ computes the *"trace"*, i.e. the sum of the diagonal terms of a tensor. $Tr(\underline{\sigma}) = \sigma_{xx} + \sigma_{yy} + \sigma_{zz}$.

The operator $\underline{dev}()$ extracts the *"deviatoric"* part. This one is the complement of the part *"spherical"* which is $\frac{1}{3}Tr()\underline{Id}$. $\underline{dev}(\underline{\sigma}) = \underline{\sigma} - \frac{1}{3}Tr(\underline{\sigma})\underline{Id}$ where $\underline{Id}$ is the *"identity tensor"* such that $Id_{xx} = 1, Id_{yy} = 1, Id_{zz} = 1, Id_{xy} = 0, Id_{xz} = 0, Id_{yx} = 0, Id_{zx} = 0, Id_{yz} = 0, Id_{zy} = 0$.

Appendix B. Meaning of the determinant of the Jacobian matrix

Appendix B.1. Volume variation and determinant of a 3D Jacobian matrix

Appendix B.1.1. Mixed product

Consider any three vectors $\overrightarrow{Ox_a}, \overrightarrow{Oy_a}, \overrightarrow{Oz_a}$. The volume V defined by the parallelepiped (O, x_a, y_a, z_a) is calculated by the mixed product:

$$V(O, x_a, y_a, z_a) = (\overrightarrow{Ox_a} \wedge \overrightarrow{Oy_a}).\overrightarrow{Oz_a} \tag{B.1}$$
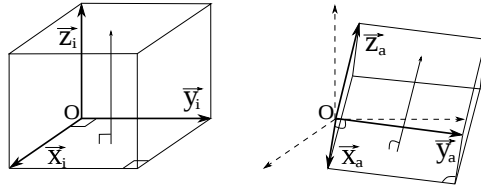

Figure B.20: Calculation of the volume of a parallelepiped by the mixed product.

Appendix B.1.2. Volume change

Let us now consider a matrix $\underline{\underline{F}}$ which transforms the vectors $\overrightarrow{OP_i}$ defined by the initial positions P_i into vectors $\overrightarrow{OP_a}$ defined by the current positions P_a.

$$\underline{\underline{F}} = \begin{bmatrix} F_{xx} & F_{xy} & F_{xz} \\ F_{yx} & F_{yy} & F_{yz} \\ F_{zx} & F_{zy} & F_{zz} \end{bmatrix} = \begin{bmatrix} \frac{\partial x_a}{\partial x_i} & \frac{\partial x_a}{\partial y_i} & \frac{\partial x_a}{\partial z_i} \\ \frac{\partial y_a}{\partial x_i} & \frac{\partial y_a}{\partial y_i} & \frac{\partial y_a}{\partial z_i} \\ \frac{\partial z_a}{\partial x_i} & \frac{\partial z_a}{\partial y_i} & \frac{\partial z_a}{\partial z_i} \end{bmatrix}$$

We have therefore for the transformation of $\overrightarrow{Ox_i} = [x_i, 0, 0]$:

$$\overrightarrow{Ox_a} = \underline{\underline{F}}\,\overrightarrow{Ox_i} = x_i \begin{bmatrix} \frac{\partial x_a}{\partial x_i} \\ \frac{\partial y_a}{\partial x_i} \\ \frac{\partial z_a}{\partial x_i} \end{bmatrix} = x_i \begin{bmatrix} F_{xx} \\ F_{yx} \\ F_{zx} \end{bmatrix} \tag{B.2}$$

We can also consider $\overrightarrow{Oy_i} = [0, y_i, 0]$ and $\overrightarrow{Oz_i} = [0, 0, z_i]$. If we now pose $x_i = y_i = z_i = 1$, then the initial volume V_i of reference defined by $[1, 1, 1]$ in an orthonormal frame of reference is 1. This unit volume is transformed by $\underline{\underline{F}}$ into an actual parallelepiped volume V_a defined by the three vectors $[F_{xx}, F_{yx}, F_{zx}]$, $[F_{xy}, F_{yy}, F_{zy}]$ and $[F_{xz}, F_{yz}, F_{zz}]$ which are respectively the transforms of $[1, 0, 0]$, $[0, 1, 0]$ and $[0, 0, 1]$ by $\underline{\underline{F}}$. Let's calculate this current volume using the mixed product:

$$V(O, x_a, y_a, z_a)_{x_i=1, y_i=1, z_i=1} = ([F_{xx}, F_{yx}, F_{zx}] \wedge [F_{xy}, F_{yy}, F_{zy}]).[F_{xz}, F_{yz}, F_{zz}]$$

$$= F_{xz}F_{yx}F_{zy} - F_{xz}F_{zx}F_{yy} + F_{yz}F_{zx}F_{xy} - F_{yz}F_{xx}F_{zy} + F_{zz}F_{xx}F_{yy} - F_{zz}F_{yx}F_{xy}$$

$$= det.\underline{\underline{F}} = \frac{V_a}{V_i} \tag{B.3}$$

where V_i denotes the initial volume and V_a denotes the current volume. It is therefore clear that physically we must check $det.\underline{\underline{F}} > 0$. For a surface, we consider for example that $\|\overrightarrow{Oz_i}\| = \|\overrightarrow{Oz_a}\| = 1$ is the unit of thickness and that $\overrightarrow{Oz_a} \perp plane(O, x_a, y_a)$ and we find well:

$$\overrightarrow{Ox_a} \wedge \overrightarrow{Oy_a} = surface(O, x_a, y_a)$$

Appendix C. Special elements, example for the singularity of fracture mechanics

An introduction to fracture mechanics can be found in [1]. For accurate fracture mechanics computation, the estimation of crack top fields must be well treated. In linear elasticity, these have a singularity in $r^{-1/2}$ where r is the distance to the crack top. Special elements must therefore be used to describe this type of evolution. Sometimes the solution consists in using cleverly already existing elements. For example, for plane or axisymmetric problems, one can use the classical 8-node quadrilaterals available in the element libraries of the calculation codes [2] [3] [4]. It is sufficient to degenerate the quadrilateral by superimposing three nodes on the crack top and to move the intermediate nodes so that the interpolation functions adopt the desired singular variation. Fig. C.21 shows the principle. However, we must be aware that we are forcing the singularity to vary as the specific element chosen. In other words, we must be sure that the solution of the problem admits the type of variation imposed by the element.
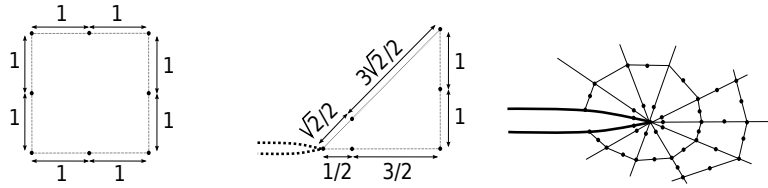
Figure C.21: Use of a classical element to treat a singularity.

Appendix D. Relation displacements - strain tensor

In two dimensions, for a four-node quadrilateral, the transpose of the gradient tensor of the displacement vector $\begin{bmatrix} u \\ v \end{bmatrix}$, denoted by $\underline{\underline{grad^T}}$, is therefore given by:

$$\underline{\underline{grad^T}}(\begin{bmatrix} u \\ v \end{bmatrix}) = \begin{bmatrix} \frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} \\ \frac{\partial v}{\partial x} & \frac{\partial v}{\partial y} \end{bmatrix} = \begin{bmatrix} J_{11} & J_{12} \\ J_{21} & J_{22} \end{bmatrix} \begin{bmatrix} N_{ia} & N_{ja} & N_{na} & N_{ma} \\ N_{ib} & N_{jb} & N_{nb} & N_{mb} \end{bmatrix} \begin{bmatrix} u_i & v_i \\ u_j & v_j \\ u_n & v_n \\ u_m & v_m \end{bmatrix}$$
(D.1)

The tensor of deformations in the plane is given by:

$$\underline{\underline{\epsilon}} = \frac{1}{2}\underline{\underline{grad}}(\begin{bmatrix} u \\ v \end{bmatrix}) + \frac{1}{2}\underline{\underline{grad^T}}(\begin{bmatrix} u \\ v \end{bmatrix}) = \begin{bmatrix} \epsilon_{xx} & \epsilon_{xy} \\ \epsilon_{xy} & \epsilon_{yy} \end{bmatrix}$$
(D.2)

$\underline{\underline{\epsilon}}$ is therefore symmetrical by construction.

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