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# NUMERICAL SOLUTION OF PARTIAL DIFFERENTIAL EQUATION PROBLEMS IN NONLINEAR MECHANICS BY QUADRATIC MINIMIZATION METHODS

by

# R. GLOWINSKI and P. LE TALLEC

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## 1. Introduction. Synopsis

The solution of the Nonlinear Partial Differential Equation Proplems arising from Physics and Continuum Mechanics has always been an important source of challenging problems for both pure and applied mathematicians. Since the second world war the numerical solution of these problems has motivated the design of computers oriented to scientific applications. Despite the impressing progresses of these computing machines (measured in terms of speed, memory, programming facilities, reliability, size, cost,...) the advanced applied problems to be solved numerically have always required to work very close the limit of the possibilities of these computers (and in fact beyond). This situation has motivated an important effort for developping efficient numerical methods for solving the above applied problems. In this direction, an important concept is the concept of decomposition, the general principle of decomposition methods being to split the original problem in problems of smaller size and/or easier to solve, and then coordinate the local results. The coordination can be done via a least squares fitting (see Secs. 1 and 2), or by Lagrange multipliers (see Secs. 4 and 5). Domain decomposition methods (such as the Schwarz alternating method), or Alternating Direction methods founded on operator splitting provide other examples of decomposition methods. For very complicated problems, we may have to use combinations of the above methods.

The main goal of this paper is to describe the numerical treatment of large highly <u>nonlinear</u> two or three dimensional boundary value problems (originating from <u>Nonlinear Mechanics</u>), by <u>quadratic minimization techniques</u>. These techniques have been applied to the solution of problems of practical interest and their principles are discussed in [6] and [7]. In all the different situations where these techniques have been applied, the methodology remains the same and is organized as follows:

- (i) Derive a variational formulation of the original boundary value problem, and approximate it by Galerkin methods;
- (ii) Transform this variational formulation into a quadratic minimization problem (<a href="least squares methods">least squares methods</a>) or into a sequence of quadratic minimization problems (augmented lagrangian decomposition);
- (iii) Solve each quadratic minimization problem by either a direct method or a conjugate gradient algorithm with preconditioning, the preconditioning matrix being sparse, positive definite, and fixed once and for all in the iterative process.

In this paper we will illustrate the above methodology by the numerical treatment of two classes of nonlinear problems: Firstly, the description of least squares solution methods and their application to the solution of the unsteady Navier-Stokes equations for incompressible viscous fluids, secondly the description of augmented lagrangian decomposition techniques and their applications to the solution of equilibrium problems in finite elasticity.

### 2. Least squares solution of a nonlinear model problem

In order to introduce the techniques which lead to the solution of nonlinear boundary value problems by least squares and conjugate gradient methods, we shall consider, first, the solution of a simple nonlinear Dirichlet problem. In section 3, these methods will then be applied to the solution of the unsteady Navier-Stokes equations for incompressible viscous fluids.

# 2.1. Formulation of the model problem

Let  $\Omega\subset \mathbb{R}^N$  be a bounded domain with a smooth boundary  $\Gamma=\partial\Omega$ ; let T be a nonlinear operator from  $V=H^1_0(\Omega)$  to  $V^*=H^{-1}(\Omega)$ ,  $V^*$  being the topological dual space of V. Standard notations are used for

Sobolev spaces (cf. [19]); in particular,  $H_0^1(\Omega)$  denotes the space of those real valued functions defined over  $\Omega$ , square-integrable, with square integrable first order derivatives and zero trace on  $\Gamma$ .

The nonlinear Dirichlet model problem is then

(2.1) 
$$\begin{cases} \frac{\text{Find } u \in H_0^1(\Omega) & \text{such that} \\ -\Delta u - T(u) = 0 & \underline{\text{in}} & H^{-1}(\Omega) \end{cases}.$$

We observe that  $u \in H_0^1(\Omega)$  implies that the trace of u on  $\Gamma$  vanishes; (2.1) is therefore a Dirichlet problem. We do not discuss here the existence and uniqueness properties of the solution of (2.1) since we do not want to be very specific about operator T.

# 2.2. $\mbox{H}^{-1}$ least squares formulation of the model problem (2.1)

Many least squares formulation of the above model problem can be proposed. Among them, a natural one, based on the norm which appears naturally in (2.1), consists to say that the solutions of (2.1) cancel the norm of  $\Delta u + T(u)$  in  $H^{-1}(\Omega)$ , and therefore minimize this norm over  $H^1_0(\Omega)$ . The least squares formulation of (2.1) is then

(2.2) 
$$\min_{\mathbf{v} \in H_0^1(\Omega)} ||\Delta \mathbf{v} + \mathbf{T}(\mathbf{v})||_{-1} ,$$

where the  $H^{-1}(\Omega)$ -norm,  $|| . ||_{-1}$ , is defined by duality, i.e.

$$||f||_{-1} = \sup_{\substack{v \in H_0^1(\Omega) \\ ||v||_{H_0^1(\Omega)}}} ,$$

where <.,.> denotes the duality pairing between  $H^{-1}(\Omega)$  and  $H^1_0(\Omega)$ , such that

$$\langle f, v \rangle = \int_{\Omega} f v \, dx \quad \forall f \in L^{2}(\Omega), \forall v \in H_{0}^{1}(\Omega).$$

Since the Laplace operator  $\Delta$  is an isometry between  $H_0^1(\Omega)$  and  $H^{-1}(\Omega)$  we can reformulate (2.2) as follows:

(2.3) 
$$\min_{\mathbf{v} \in H_0^1(\Omega)} ||\Delta^{-1}(\Delta \mathbf{v} + \mathbf{T}(\mathbf{v}))||^2 H_0^1(\Omega) .$$

Taking into account the definition of the  $H_0^1(\Omega)$ -norm we introduce the function  $\xi(v)$ , defined from v by

(2.4) 
$$\Delta \xi = \Delta v + T(v) \quad \underline{in} \quad H^{-1}(\Omega), \quad \xi \in H_0^1(\Omega),$$

with  $\xi = \xi(v)$ . Thus  $\xi(=\xi(v))$  is obtained from v, via the solution of a <u>linear Dirichlet problem</u> whose <u>variational</u> formulation (equivalent to (2.4)) is given by

$$(2.5) \quad \xi \in H_0^1(\Omega), \quad \int_{\Omega} \nabla \xi \cdot \nabla w \, dx = \int_{\Omega} \nabla v \cdot \nabla w \, dx - \langle T(v), w \rangle \quad \forall w \in H_0^1(\Omega).$$

Using  $\xi(v)$  the minimization problem (2.2) can be written also as follows :

(2.6) 
$$\operatorname{Min}_{\mathbf{v} \in H_{0}^{1}(\Omega)} \left\{ \frac{1}{2} \int_{\Omega} \left| \nabla \xi(\mathbf{v}) \right|^{2} d\mathbf{x} \right\}$$

with  $\xi(v)$  solution of (2.4), (2.5). Using (2.6) we have obtained a minimization formulation of the initial problem (2.1); combining (2.6) to the conjugate gradient algorithm described in Sec. 2.3, below, the solution of (2.1) will be reduced to that of a sequence of linear problems associated to the Laplace operator  $\Delta$ .

We observe that (2.6) has the structure of an optimal control problem (see [20]) where v is the control vector,  $\xi$  the state vector, (2.5) the state equation, and where the functional  $J: H_0^1(\Omega) \to \mathbb{R}$  defined by

$$J(v) = \frac{1}{2} \int_{\Omega} |\nabla \xi(v)|^2 dx$$

is the cost function.

2.3. Conjugate gradient solution of the least squares problem (2.6).
Problem (2.6) is a minimization problem. For its solution we shall use a conjugate gradient algorithm. Due to its good performances, (cf. [22],[23]), we have selected the Polak-Ribière version of the conjugate gradient method, that is:

# Step 0 : Initialization

(2.7) 
$$u^{\circ} \in H_0^1(\Omega) \quad \underline{given},$$

compute then  $g^{\circ} \in H_0^1(\Omega)$  as the solution of

$$-\Delta g^{\circ} = J'(u^{\circ}) \quad \text{in } H^{-1}(\Omega),$$

and set

$$(2.9) z^{\circ} = q^{\circ}.$$

Then for  $n \ge 0$ , assuming  $u^n$ ,  $g^n$ ,  $z^n$  known, compute  $u^{n+1}$ ,  $g^{n+1}$ ,  $z^{n+1}$  by

# Step 1 : Descent

(2.10) 
$$u^{n+1} = u^n - \lambda_n z^n$$
,

where  $\lambda_n$  is the solution of the one-dimensional minimization problem

$$\begin{cases} \lambda_n \in \mathbb{R}, \\ J(u^n - \lambda_n z^n) \leq J(u^n - \lambda z^n) \quad \forall \lambda \in \mathbb{R}. \end{cases}$$

# 

(2.12) 
$$-\Delta g^{n+1} = J'(u^{n+1}) \text{ in } H^{-1}(\Omega),$$

and set

(2.13) 
$$\gamma_{n} = \int_{\Omega} \nabla g^{n+1} \cdot \nabla (g^{n+1} - g^{n}) dx / \int_{\Omega} |\nabla g^{n}|^{2} dx ,$$

(2.14) 
$$z^{n+1} = g^{n+1} + \gamma_n z^n$$
.

# Go back to Step 1 with n = n+1.

The two non trivial steps of algorithm (2.7)-(2.14) are:

(i) The solution of the single variable minimization problem (2.11); the corresponding line search can be achieved by dichotomy or Fibonacci methods. Observe that each evaluation of J(v) for a given

argument v requires the solution of the linear Poisson problem (2.4), (2.5) to obtain the corresponding  $\boldsymbol{\xi}$  .

(ii) The calculation of  $g^{n+1}$  from  $u^{n+1}$  which requires the solution of two linear Poisson problems, namely (2.4), (2.5) with  $v = u^{n+1}$ , and (2.12).

Let us detail the calculation of  $g^{n+1}$ . By construction of J we have

$$= \int_{\Omega} \underbrace{\nabla}_{\Sigma} \xi(v) \cdot \underbrace{\nabla}_{\Sigma} \eta(v, w) dx \quad \forall w \in H_{0}^{1}(\Omega),$$

with  $\eta(v, w) (= \eta)$  solution of

$$\eta \in H_0^1(\Omega)$$
,  $\Delta \eta = \Delta w + T'(v).w in  $H^{-1}(\Omega)$ .$ 

After elimination of  $\eta$  we obtain

$$\langle J'(v), w \rangle = \int_{0}^{\infty} \nabla \xi(v) \nabla w dx - \langle T'(v), w, \xi(v) \rangle \quad \forall v, w \in H_0^1(\Omega).$$

Thus problem (2.12) reduces to the following linear variational (Poisson) problem

$$\begin{cases} \frac{\text{Find }}{\sigma} g^{n+1} \in H_0^1(\Omega) & \underline{\text{such that}} \ \forall w \in H_0^1(\Omega) \text{, we have} \\ \int_{\Omega} \overline{y} g^{n+1} \cdot \overline{y} w dx = \int_{\Omega} \overline{y} \xi^{n+1} \cdot \overline{y} w dx - \langle T'(u^{n+1}) \cdot w, \xi^{n+1} \rangle, \end{cases}$$

where  $\xi^{n+1}$  is the solution of (2.4), (2.5) corresponding to  $v = u^{n+1}$ .

Remark 2.1. : As stopping criterion for the conjugate gradient algorith (2.7)-(2.14) we shall use

$$\mathtt{J}\left(\mathtt{u}^{n}\right) \;\; \leq \;\; \epsilon \qquad \underline{\mathtt{or}} \qquad \left|\left|\,\mathtt{g}^{\,n}\,\right|\right| \;\; _{H^{\,1}_{\,0}\left(\Omega\right)} \;\; \leq \;\; \epsilon$$

where  $\epsilon$  is a reasonably small positive number.

Remark 2.2.: It is clear from the above observations that an efficient Poisson solver is the basic tool for solving the model problem (2.1) by our conjugate gradient algorithm. Any size limitation for this algorithm will come from a limitation on the Poisson solver.

Remark 2.3.: The above methodology (possibly combined to arc length continuation methods; cf. [8]) extends easily to the solution of

many other nonlinear boundary value problems: Von Karman equations for thin clamped plates (cf. [24]), transonic flow problems (cf. [8], []), etc... The choice of (2.1) as a model problem was only made for clarity reasons. In the next section we shall apply this methodology to the solution of the nonlinear elliptic system

$$\alpha u - \nu \Delta u + (u.\nabla) u = f \underline{in} \Omega$$
,

with u a vector valued function, defined a.e. on  $\Omega$ , with values in  $\mathbb{R}^N$ . Such a nonlinear system is closely related to the solution of the time dependent Navier-Stokes equations by alternating direction methods.

- 3. <u>Application to the solution of the Navier-Stokes equations for in-</u>compressible viscous fluids.
- 3.1. Formulation of the time dependent Navier-Stokes equations for incompressible viscous fluids.

Let us consider a newtonian incompressible viscous fluid; if  $\Omega$  and  $\Gamma$  denote the region of the flow ( $\Omega \subset \mathbb{R}^N$ , N=2 or 3 in practice) and its boundary, respectively, then this flow is governed by the Navier-Stokes equations which relate velocity and pressure inside the fluid to the external sources of motion (initial velocity, motion of the boundary, external forces, etc...); these equations are given by

(3.1) 
$$\begin{cases} \frac{\partial \mathbf{u}}{\partial \mathbf{t}} - \nabla \Delta \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} + \nabla \mathbf{p} &= \mathbf{f} \quad \underline{\mathbf{in}} \quad \Omega \\ \nabla \cdot \mathbf{u} &= 0 \quad \underline{\mathbf{in}} \quad \Omega \end{cases} \quad (\underline{\mathbf{incompressibility condition}}).$$

Above,  $u = \{u_i\}_{i=1}^N$  denotes the flow velocity, p the <u>hydrostatic pressure</u>, v the <u>viscosity</u> of the fluid, f the <u>density of external forces</u>. Moreover  $(u, \nabla)u$  is a symbolic notation for the <u>skewsymmetric quadratic</u> vector term corresponding to the convection in equation (3.1), i.e.

$$(\underbrace{u},\underbrace{\nabla})_{u} = \underbrace{\sum_{j=1}^{N} \{u_{j} \frac{\partial u_{i}}{\partial x_{j}}\}_{i=1}^{N}}.$$

To fully characterize the flow, initial and boundary conditions have to be imposed on  $\ddot{u}$ . In the case of the airfoil A of Figure 3.1, we typically have

(3.2) 
$$u(x,t) = 0$$
 on  $\partial A$  (adherence condition on the airfoil),

(3.3) 
$$u(x,t) = u_{\infty}(t)$$
 at infinity,

(3.4) 
$$\underbrace{u(x,0) = u_{0}(x) \text{ (initial condition)}}_{\infty}.$$



Figure 3.1.

For a flow in a bounded region  $\Omega$  of  ${\rm I\!R}^N$ , we may replace the boundary conditions (3.2), (3.3) by

(3.5) 
$$u(x,t) = g(x,t)$$
 on  $\Gamma$ .

where due to the incompressibility condition  $\nabla \cdot u = 0$ , the given function g must satisfy

$$\int_{\Gamma} \underbrace{g.n}_{\cdot} d\Gamma = 0 \quad (n_{\cdot}: \text{ unit vector normal to } \Gamma).$$

In the above equations the main difficulties are

- (i) The nonlinear term  $(u.\nabla)u$  in (3.1);
- (ii) The incompressibility condition  $\nabla \cdot u = 0$ .

Using convenient <u>alternating direction methods</u> for the <u>time discretization</u> of the Navier-Stokes equations, we shall be able to decouple these difficulties; problem (3.1), (3.5), (3.4) will reduce then to a sequence of

- (a) Incompressible linear problems,
- (b) Compressible nonlinear problems to be solved by the least squaresconjugate gradient methods of Sec. 2, that is via the solution of a sequence of strongly elliptic linear problems.

All the resulting linear problems will be associated (via a suitable space discretization) to fixed matrices. Ad hoc algorithms can

then be deviced for their numerical solution, even for large size problems. At this stage <u>multigrid</u> methods (cf. [15]) or <u>domain decomposition</u> methods (cf. [5]) (or a combination of both) become very attractive.

# 3.2. Time discretization by alternating direction methods.

For simplicity, we suppose from now on that  $\Omega$  is <u>bounded</u>. Let  $\Delta t > 0$  be a time discretization step. The alternating direction method that is found to be the most convenient computationaly, to discretize (3.1), (3.5), (3.4) is described just below:

$$(3.6) \underline{\text{Let}} \ \underline{\mathbf{u}}^{\mathsf{O}} = \underline{\mathbf{u}} \ ;$$

then for  $n \ge 0$ , and starting from  $u^n$ , we solve successively

(3.7) 
$$\begin{cases} \frac{u^{n+1/4} - u^n}{\Delta t/4} - 2 \frac{v}{3} \Delta u^{n+1/4} + \frac{v}{v} p^{n+1/4} \\ = f^{n+1/4} + \frac{v}{3} \Delta u^n - (u^n \cdot v) u^n & \underline{in} \quad 0, \\ v \cdot u^{n+1/4} = 0 & \underline{in} \quad 0, \\ u^{n+1/4} = g^{n+1/4} & \underline{on} \quad \Gamma, \end{cases}$$

$$\begin{cases} \frac{u^{n+3/4} - u^{n+1/4}}{\Delta t/2} - \frac{v}{3} \Delta u^{n+3/4} + (u^{n+3/4} \cdot v) u^{n+3/4} = \\ \frac{f^{n+3/4} - v}{\Delta t/2} - \frac{v}{3} \Delta u^{n+1/4} & \underline{in} \quad 0, \\ u^{n+3/4} = g^{n+3/4} & \underline{on} \quad \Gamma, \end{cases}$$

$$\begin{cases} \frac{u^{n+1} - u^{n+3/4}}{\Delta t/4} - 2 \frac{v}{3} \Delta u^{n+1} + v p^{n+1} = \\ \frac{v^{n+1} - u^{n+3/4}}{\Delta t/4} - 2 \frac{v}{3} \Delta u^{n+1/4} & \underline{v} \cdot v^{n+3/4} = 0 \end{cases}$$

$$\begin{pmatrix}
\frac{u^{n+1} - u^{n+3/4}}{\Delta t/4} - 2 \frac{v}{3} \Delta u^{n+1} + \nabla p^{n+1} = \\
\frac{f^{n+1}}{\Delta t/4} + \frac{v}{3} \Delta u^{n+3/4} - (u^{n+3/4} \cdot \nabla) u^{n+3/4} & \underline{in} \Omega, \\
\nabla \cdot u^{n+1} = 0 & \underline{in} \Omega, \\
u^{n+1} = g^{n+1} & \underline{on} \Gamma.
\end{pmatrix}$$

The notation  $f^j(x)$  and  $g^j(x)$  denote  $f(x,j\Delta t)$  and  $g(x,j\Delta t)$ , respectively;  $u^j(x)$  is an approximation for  $u(x,j\Delta t)$ .

Remark 3.1. Due to the symmetrization process that it involves, scheme (3.7)-(3.9) has a truncation error of  $0(|\Delta t|^2)$ . Although the linear step (3.7) and (3.9) are identical, suppressing one of them would not be adviseable: it would increase the truncation error with no real gain on the computational time, which is mainly devoted to the nonlinear step (3.8).

Remark 3.2. : The decomposition of the operator -  $\nu\Delta u$  between the right and left hand sides of equations (3.7), (3.8), (3.9) was done in order to involve the same linear operators in each step; this strategy results in quite substantial computer core memory savings.

Remark 3.3. : We have introduced the alternating direction decomposition of (3.1) for the continuous problems, since their formalism is simpler. But, of course, the same decomposition would apply to any Galerkin approximation of the Navier-Stokes equations, obtained by finite element methods, for example (see [7, Chapter 7]); actually the combination of the above alternating direction methods with spectral methods of approximation is under test at the moment (the corresponding results will be published elsewhere).

Remark 3.4. : Related operator splitting methods for the Navier-Stokes equations are discussed in [1].

3.3. Least squares conjugate gradient solution of the nonlinear subproblems (3.8).

At each full step of the alternating direction method (3.7)-(3.9) we have to solve a nonlinear elliptic problem of the following type

(3.10) 
$$\begin{cases} \alpha \overset{\cdot}{u} - \nu \Delta \overset{\cdot}{u} + (\overset{\cdot}{u} \cdot \overset{\cdot}{\nabla}) \overset{\cdot}{u} = \overset{f}{\kappa} & \underline{i}\underline{n} & \Omega \\ \overset{\cdot}{u} = \overset{\cdot}{g} & \text{on} & \Gamma. \end{cases}$$

Once the Laplace operator of Sec. 2 has been replaced by the operator  $\alpha I$  -  $\nu \Delta$ , applying to (3.10) the least squares methodology of Sec. 2 yields the following minimization problem

where

$$J(\underline{v}) = \frac{1}{2} \int_{\Omega} \{\alpha | \underline{y}(\underline{v}) |^2 + \nu | \underline{\nabla} \underline{y}(\underline{v}) |^2 \} dx,$$

and where y(v) (=y) is the only solution of

(3.13) 
$$\begin{cases} \tilde{y} \in V_{O} \\ \alpha \tilde{y} - \nu \Delta \tilde{y} = \alpha \tilde{v} - \nu \Delta \tilde{v} + (\tilde{v} \cdot \tilde{v}) \tilde{v} - \tilde{t} & \underline{\text{in}} V_{O}^{*}; \end{cases}$$

the space  $V_{\Omega}$  and the set  $V_{\alpha}$  are defined by

$$V_{o} = (H_{0}^{1}(\Omega))^{N}, V_{g} = \{ \underline{v} | \underline{v} \in (H^{1}(\Omega))^{N}, \underline{v} = \underline{g} \quad \underline{on} \quad \Gamma \}$$

respectively, and  $V_{O}^{\star}$  is the topological dual space of  $V_{O}^{\star}$ .

Thus, the solution of subproblems (3.8), in the alternating direction time discretization of the Navier-Stokes equations, reduces to the solution of the minimization problem (3.11); such a minimization can be achieved by conjugate gradient methods and particularly by a Polak-Ribière algorithm, like in Sec. 2. Compared to algorithm (2.7)-(2.14), -  $\Delta$  will have to be replaced by  $\alpha I - \nu \Delta$ ; in particular we should replace the calculation of  $g^{n+1}$  in (2.12) by

$$\begin{cases} \underbrace{\text{Find }}_{\Omega} \overset{\circ}{\mathbb{g}}^{n+1} \in V_{O} & \underline{\text{such that }}_{W} \in V_{O} & \underline{\text{we have}} \\ \int_{\Omega} \{\alpha \overset{\circ}{\mathbb{g}}^{n+1} \cdot \overset{\circ}{\mathbb{w}} + \nu \overset{\circ}{\mathbb{v}} \overset{\circ}{\mathbb{g}}^{n+1} \cdot \overset{\circ}{\mathbb{v}} \overset{\circ}{\mathbb{w}} \} & dx = \int_{\Omega} \{\alpha \overset{\circ}{\mathbb{y}}^{n+1} \cdot \overset{\circ}{\mathbb{w}} \\ + \nu \overset{\circ}{\mathbb{v}} \overset{\circ}{\mathbb{y}}^{n+1} \cdot \overset{\circ}{\mathbb{v}} \overset{\circ}{\mathbb{w}} \} & dx + \int_{\Omega} \{\overset{\circ}{\mathbb{y}}^{n+1} \cdot (\overset{\circ}{\mathbb{w}} \cdot \overset{\circ}{\mathbb{v}}) \overset{\circ}{\mathbb{u}}^{n+1} + \overset{\circ}{\mathbb{y}}^{n+1} \cdot (\overset{\circ}{\mathbb{u}}^{n+1} \cdot \overset{\circ}{\mathbb{v}}) \overset{\circ}{\mathbb{w}} \} dx \end{cases}$$

where  $y^{n+1} = y(u^{n+1})$ .

Each iteration of the conjugate gradient algorithm applied to the solution of (3.11) finally requires the solution of four linear systems associated to the operator  $\alpha I - \nu \Delta$  , that is

- sociated to the operator  $\alpha \text{I}-\nu \Delta$  , that is (i) One for computing  $y_{i}^{n+1}$  (=  $y_{i}(y_{i}^{n+1})$ ) through (3.13),
- (ii) One for computing  $g^{n+1}$  through (3.14),
- (iii) Two to obtain the coefficients of the quartic polynomial

$$\lambda \rightarrow J(u^n - \lambda w^n)$$
.

In practice, the solution of the one-dimensional line search problem can be done very efficiently since it is equivalent to finding the

roots of a single variable <u>cubic polynomial</u> whose coefficients are known. The solution of each system associated to  $\alpha I - \nu \Delta$  corresponds to the solution of N independent scalar Dirichlet problems associated to the same operator. The conjugate gradient algorithm appears then to be very efficient in this situation: usually three iterations suffice to reduce the cost function by a factor of  $10^4$  to  $10^6$ . Therefore the whole solution of problem (3.8) by the techniques discussed in the present section is not costly, nor for its implementation, neither for its computational running time.

# 3.4. Solution of the quasi-Stokes problems (3.7) and (3.9).

These linear equations, which appear at each full step of the alternating direction method (3.7)-(3.9), involve two unknowns (<u>velocity</u> and <u>pressure</u>) and are of the following type:

(3.15) 
$$\begin{cases} \alpha \overset{\cdot}{u} - \nu \Delta \overset{\cdot}{u} + \overset{\cdot}{\nabla} p = \overset{f}{\chi} & \underline{in} & \Omega, \\ \overset{\cdot}{\nabla} \cdot \overset{\cdot}{u} = 0 & \underline{in} & \Omega, & \overset{\cdot}{u} = \overset{g}{\chi} & \underline{on} & \Gamma. \end{cases}$$

Many existing solvers can be used for this problem (once a suitable space approximation has been done) : they can be direct methods such as Gaussian elimination (via an LU factorization), Cholesky factorization if (3.15) is approximated by a Galerkin method in which the basis functions are also divergence free (exactly or approximately), property which allows the elimination of p in (3.15) and yields a finite dimensional linear system whose matrix is symmetric and positive definite (see [16] for more details). One can think also to other methods for solving (3.15) such as augmented lagrangian methods (closely related to the methods discussed in Secs. 4 and 5); decomposition methods including the solution of a boundary integral problem, related to the trace of p on \(\Gamma\), can also be used (see, e.g. [7, Chapter 7]) leading to quite efficient Stokes solvers. Actually we can solve (3.15) (or its discrete variants) by a conjugate gradient algorithm quite easy to implement since it reduces the solution of (3.15) to a sequence of scalar Dirichlet problems for  $\alpha \text{I-v}\Delta$  ; let detail this algorithm (we still suppose that  $\Omega$  is bounded in  $\mathbb{R}^{N}$ ).

We introduce first the space  $H \subset L^2(\Omega)$  by

(3.16) 
$$H = \{q | q \in L^{2}(\Omega), \int_{\Omega} q(x) dx = 0\}$$

and then  $\mathcal{T}: H \to H$  by

(3.17) 
$$\begin{cases} \alpha \underset{\sim}{\mathbf{u}}_{\mathbf{q}} - \nu \Delta \underset{\sim}{\mathbf{u}}_{\mathbf{q}} = - \nabla \mathbf{q} & \underline{\mathbf{in}} \ \Omega \end{cases},$$

$$\mathbf{u}_{\mathbf{q}} = \underbrace{\mathbf{0}}_{\mathbf{q}} & \underline{\mathbf{on}} \ \Gamma \end{cases},$$

$$\mathcal{L}_{\mathbf{q}} = \mathbf{v} \cdot \mathbf{u}_{\mathbf{q}} \quad \forall \mathbf{q} \in \mathbf{H} .$$

It is easy to check that  $\mathcal{B}$  is an <u>automorphism from H</u> onto itself, which is <u>symmetric</u> and H-elliptic (this last property meaning the existence of  $\beta>0$  such that

$$\int_{\Omega} (x^{2}q) q \, dx \geq \beta ||q||^{2} L^{2}(\Omega) \quad \forall q \in H).$$

We introduce now  $\underset{\sim}{u} \in V_q$  as the solution of

(3.19) 
$$\begin{cases} \alpha \underline{u}_{0} - \nu \Delta \underline{u}_{0} = \underline{f} & \underline{i}\underline{n} & \Omega, \\ \underline{u}_{0} = \underline{g} & \underline{o}\underline{n} & \Gamma. \end{cases}$$

Back to (3.17) we consider the unique pair  $\{u,p\}$  solution of (3.17) such that p  $\epsilon$  H ; we have then

(3.20) 
$$\begin{cases} \alpha \left( u - u_{O} \right) - \nu \Delta \left( u - u_{O} \right) + \nabla p = 0 \\ u - u_{O} = 0 & \underline{on} \Gamma \end{cases}$$

implying, from (3.15), (3.16) that

$$\mathcal{A}_{p} = \nabla (\mathbf{u} - \mathbf{u}_{0})$$
,

which reduces, since  $\nabla .u = 0$  to

From the properties of  $\mathcal{R}$  it is tempting to solve (3.21) (and therefore (3.17)) by a conjugate gradient algorithm; we first consider the abstract form of such an algorithm

# Step 0 : Initialization

(3.22) 
$$p^{\circ} \in H$$
 is given arbitrarily  $(p^{\circ} = 0 \text{ for example})$ 

$$(3.24) w^{\circ} = g^{\circ} . \qquad \Box$$

Then for  $n \ge 0$ , with  $p^n$ ,  $q^n$ ,  $w^n$  known, we obtain  $p^{n+1}$ ,  $q^{n+1}$ ,  $w^{n+1}$  as follows :

$$\frac{\text{follows}:}{\text{Step 1}: \underline{\text{Descent}}} \\ (3.25) \qquad \rho_n = \frac{\|\mathbf{g}^n\|_{L^2(\Omega)}^2}{(\mathbf{k}_w^n, \mathbf{w}^n)_{L^2(\Omega)}},$$

(3.26) 
$$p^{n+1} = p^n - \rho_n w^n$$
.

Step 2 : New descent direction

(3.27) 
$$g^{n+1} = g^n - \rho_n \mathcal{A}_w^n$$
,

(3.28) 
$$\gamma_{n} = \frac{||g^{n+1}||_{L^{2}(\Omega)}^{2}}{||g^{n}||_{L^{2}(\Omega)}^{2}} ,$$

(3.29) 
$$w^{n+1} = g^{n+1} + \gamma_n w^n$$
.

Do n = n+1, go back to (3.25).

Actually since operator  $\mathcal X$  is not known explicitely we should proceed as follows in practice :

With  $p^{O}$  as in (3.22), compute  $u^{O} \in V_{q}$  by solving

(3.30) 
$$\begin{cases} \alpha \underline{u}^{\circ} - \nu \Delta \underline{u}^{\circ} = \underline{f} - \nabla \underline{p}^{\circ} & \text{in } \Omega, \\ \underline{u}^{\circ} = \underline{g} & \underline{on} & \Gamma, \end{cases}$$

and set

$$(3.31) g^{\circ} = \nabla . u^{\circ},$$

$$(3.32)$$
  $w^{\circ} = g^{\circ}.$ 

For  $n \ge 0$ ,  $u^n$ ,  $p^n$ ,  $g^n$ ,  $w^n$  being known solve

$$\begin{cases} \alpha \chi^{n} - \nu \Delta \chi^{n} = - \nabla w^{n} \underline{in} & \Omega, \\ \chi^{n} \in V_{O} (= (H_{0}^{1}(\Omega))^{N}), \end{cases}$$

compute

(3.34) 
$$\rho_{n} = \frac{\|\mathbf{g}^{n}\|^{2}_{\mathbf{L}^{2}(\Omega)}}{\int_{\Omega} \mathbf{x} \cdot \mathbf{x}^{n} \mathbf{w}^{n} d\mathbf{x}},$$

and then

(3.35) 
$$p^{n+1} = p^n - \rho_n w^n$$
,

$$(3.36) \qquad \qquad \underbrace{u^{n+1}}_{n} = \underbrace{u^{n}}_{n} - \rho_{n} \underbrace{x}_{n}^{n} ,$$

$$(3.37) g^{n+1} = g^n - \rho_n \nabla \cdot \chi^n ,$$

(3.38) 
$$\gamma_{n} = \frac{\|g^{n+1}\|_{L^{2}(\Omega)}^{2}}{\|g^{n}\|_{L^{2}(\Omega)}^{2}} ,$$

(3.39) 
$$w^{n+1} = g^{n+1} + \gamma_n w^n ,$$

do then n = n+1 and go back to (3.33).

Remark 3.5. : The costly part of the above conjugate gradient algorithm is the solution of the Dirichlet system (3.33) ; we observe however that the N components of  $\chi^n$  can be computed independently (and possibly in parallel).

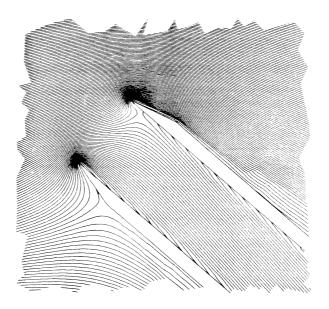
Remark 3.6. : If we do not suppose that  $p^O$  belongs to H we shall have convergence of  $\{u^n, p^n\}$  to a limit  $\{u, p\}$  which is the unique solution of (3.17) such that

$$\int_{0}^{\infty} p dx = \int_{0}^{\infty} p^{\circ} dx .$$

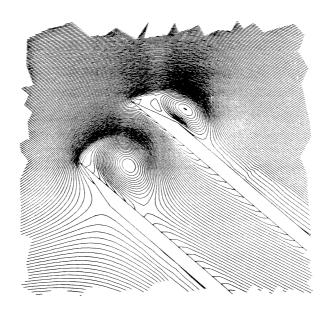
Remark 3.7.: For very large problems, when the finite element approximation of the Navier-Stokes equations involve several ten thousands of unknowns, it might be useful to split (3.13), (3.14), (3.33) into smaller size problems of the same type, obtained by domain decomposition techniques (see [5] for more details).

# 3.5. Numerical experiments.

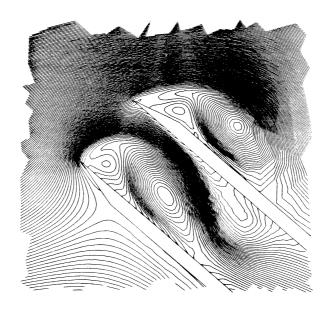
We illustrate the numerical techniques discussed in the above sections by presenting some results of numerical experiments where these techniques have been used to simulate several incompressible viscous



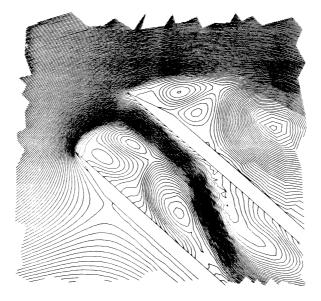
Re = 750 ; t = .0 Figure 3.2



Re = 750 ; t = .2 Figure 3.3



Re = 750 ; t = .4 Figure 3.4



Re = 750; t = .6 Figure 3.5

flows modelled by the Navier-Stokes equations.

The experiment presented here concerns an unsteady flow around and inside a nozzle at high incidence (30 degrees) and at Reynolds number 750 (the characteristic length being the distance between the nozzle walls). The finite element methods used to approximate the Navier-Stokes equations in this experiment are discussed in [ , Chapter 7]. Figures 3.2 to 3.5 represent the streamlines at t=0, t=.2, t=.4, t=.6 respectively, showing clearly the creation and motion of eddies of various scales, inside and behind the nozzle (for more results obtained by the methods in this paper see [7, Chapter 7], [5],[13]).

# 4. Decomposition Methods by Augmented Lagrangians.

The main goal of this section is to give a brief account of solution methods for variational problems when some decomposition property holds; introducing a convenient <u>augmented lagrangian</u>, we obtain solution methods taking full advantage of the special structure of the problem under consideration. We shall first consider in this section the solution by augmented lagrangians of a simple nonlinear model problem, before considering in Sec. 5 the application of these techniques to the solution of nonlinear three-dimensional problems in Finite Elasticity.

# 4.1. Formulation of the model problem

Let  $\Omega \subset \mathbb{R}^2$  be a <u>bounded</u> domain with a smooth boundary  $\Gamma = \partial \Omega$ , and consider the following model problem (with 1 ):

(4.1) 
$$\begin{cases} -\nabla \cdot (|\nabla u|^{p-2}\nabla u) = f & \underline{in} & \Omega, \\ u = 0 & \underline{on} & \Gamma_1, \\ |\nabla u|^{p-2}\nabla u \cdot \underline{n} = \underline{g} & \underline{on} & \Gamma_2; \end{cases}$$

in (4.1) we have 
$$\Gamma_1$$
  $\cap$   $\Gamma_2$  =  $\emptyset$ ,  $\Gamma_1$   $\cup$   $\Gamma_2$  =  $\Gamma$  ,  $\int$   $\Gamma_1$   $d\Gamma$  > 0.

Such problems, discussed in [14] appear for example in the study of Norton viscoplastic fluids flowing viscously in a cylindrical duct. Problem (4.1) is actually equivalent to the following problem of the Calculus of Variations:

(4.2) 
$$\begin{cases} \underline{\text{Find}} & u \in V & \underline{\text{such that}} \\ J(u) \leq J(v) & \forall v \in V \end{cases}$$

where

(4.3) 
$$V = \{v | v \in W^{1,p}(\Omega), w = 0 \text{ on } \Gamma_1\}$$

$$(4.4) J(v) = \frac{1}{p} \int_{\Omega} |\nabla v|^p dx - \int_{\Omega} fv dx - \int_{\Gamma_2} gv d\Gamma .$$

Observe now that the above functional J(.) can be naturally decomposed as follows:

We have therefore for (4.1), (4.2) the equivalent formulation

where the space W and the functional j(.) are defined (with H =  $(\mathtt{L}^p(\Omega))^N$ ) by

(4.7) 
$$W = \{\{v,G\} \mid v \in V, G \in H, G = Bv\}$$

(4.8) 
$$j(v,G) = \mathcal{F}(G) + \mathcal{G}(v),$$

respectively. Problems (4.1), (4.2) and (4.6) are indeed equivalent but (4.8) has in some sense a simpler structure than (4.1), (4.2), despite the fact it contains an extra variable. This is because the <u>linear relation Bv-G</u> = 0 can be efficiently treated by methods using simultaneously <u>penalty</u> and <u>Lagrange multipliers</u>, via an approximate augmented lagrangian (cf. [6]).

## 4.2. An augmented lagrangian associated to (4.6).

Let R be a strictly positive parameter; we define then an augmented lagrangian  $\mathcal{Z}_R$  from V × H × H\* (H\* = (LP\*)N;  $\frac{1}{p} + \frac{1}{p*} = 1$ ) into R by

$$\left\{ \begin{array}{l} \boldsymbol{\mathcal{Z}}_{R}(v,\underline{G},\underline{\mu}) = \boldsymbol{\mathcal{F}}(\underline{G}) + \boldsymbol{\mathcal{G}}(v) + \frac{R}{2} \left\| Bv - \underline{G} \right\|_{0,\Omega}^{2} + \int_{\Omega} \mu \cdot (Bv - \underline{G}) \, dx \\ = \frac{1}{p} \int_{\Omega} |\underline{G}|^{p} dx - \int_{\Omega} fv dx - \int_{\Gamma_{2}} gv d\Gamma + \int_{\Omega} \left\{ \frac{R}{2} |\underline{\nabla} v - \underline{G}|^{2} + \mu \cdot (\underline{\nabla} v - \underline{G}) \right\} dx, \\ \text{where } \|\underline{G}\|_{0,\Omega} = \|\underline{G}\|_{(L^{2}(\Omega))^{2}} \quad \forall \underline{G} \in (L^{2}(\Omega))^{2}.$$

Remark 4.1. : We have to suppose that  $p \ge 2$  in (4.9) to have  $\nabla v - G = \varepsilon (L^2(\Omega))^2 = \forall \{v,G\} \in V \times H \text{ ; however the algorithms obtained from the above } \mathbb{Z}_R^{\bullet}$  behave quite well for p < 2, once (4.1) has been approximated, even by the most standard finite element methods (see [6],[14] for more details).

Back to (4.9) we consider the problem

$$(4.10) \qquad \qquad \underline{\text{Find}} \ \{\{u,F\},\lambda\} \quad \underline{\text{saddle point of}} \ \mathcal{Z}_{R} \ \underline{\text{over}} \ \{v \times H\} \times H^*,$$

or, in other words,

Find 
$$\{\{u,F\},\lambda\}\in\{V\times H\}\times H^*$$
 such that

$$\mathcal{Z}_{R}(u,F,\lambda) \leq \mathcal{Z}_{R}(v,G,\lambda) \quad \forall \{v,G\} \in V \times H,$$

(4.12) 
$$\mathcal{Z}_{R}(u,F,\lambda) \geq \mathcal{Z}_{R}(u,F,\mu) \quad \forall \mu \in H^{*}.$$

Problems (4.10) and (4.6) are equivalent. Indeed, let  $\{\{u,F\},\lambda\}$  be a solution of (4.10). From (4.12), we have  $F = \nabla u$ , necessarily which means that  $\{u,F\} \in W$ . Then if we write (4.11) with  $\{v,G\}$  in W we obtain

$$j(u,F) \leq j(v,G) \quad \forall \{v,G\} \in W.$$

which means precisely that  $\{u, F\}$  is a solution of (4.6). Conversely, if  $\{u, F\}$  is a solution of (4.6), by denoting  $\lambda = \mathcal{F}^\bullet(F) \ (=|F|^{p-2}F)$ , one checks easily that  $\{\{u, F\}, \lambda\}$  is a solution of (4.10). Observe that in this proof, the penalty term  $\frac{R}{2} \| |Bv-G| \|_{0,\Omega}^2$  plays no role. But its role is fundamental in accelerating the convergence of the numerical algorithms used for the solution of the saddle-point problem (4.10).

# 4.3. An Uzawa algorithm for solving (4.10).

In Sec. 4.2 we have replaced the original model problem (4.1) by the equivalent saddle-point formulation (4.10). A basic algorithm for the solution of this last problem combines an Uzawa algorithm for the solution of the saddle-point problem and a block relaxation algorithm for the solution of the minimization subproblems associated to the primal variable  $\{v,G\}$ . This leads to the following algorithm

$$(4.13) {\{\chi^{\circ}, u^{-1}\} \in H^{*} \times V \text{ is given };}$$

then for  $n\geq 0$  ,  $u^{n-1}$  and  $\lambda^n$  being known, we compute  $\{u^n,\tilde{\mathbb{F}}^n\}$  by block relaxation, i.e. by setting

$$(4.14) u_0^n = u^{n-1},$$

and by computing sequentially  $\mathbf{u}_{k}^{n}$  and  $\mathbf{F}_{k}^{n}$  by solving

$$\mathcal{Z}_{\mathbb{R}}(u_{k-1}^n, F_k^n, \lambda^n) \leq \mathcal{Z}_{\mathbb{R}}(u_{k-1}^n, G, \lambda^n) \quad \forall G \in \mathbb{H} ; F_k^n \in \mathbb{H},$$

$$(4.16) \mathcal{Z}_{R}(u_{k}^{n}, \mathcal{F}_{k}^{n}, \lambda^{n}) \leq \mathcal{Z}_{R}(v, \mathcal{F}_{k}^{n}, \lambda^{n}) \quad \forall v \in V ; u_{k}^{n} \in V.$$

Once  $\{u^n, F^n\}$  known, the Lagrange multiplier  $\lambda^n$  is updated by

$$\lambda^{n+1} = \lambda^n + \rho \quad R_z(\nabla u^n - F^n), \quad \rho > 0,$$

 $R_{\overline{z}}$  being the Riesz mapping from H onto its dual space H\* (i.e.

$$R_{2}(G) = |G|^{p-2}G \quad \forall G \in H$$
).

Remark 4.2.: Many variants of the above algorithm exists; they are described in e.g., [6].

Remark 4.3. : In practice, once problem (4.1) has been approximated by a convenient finite element method, we should replace  $R_Z$  by the <u>Identity mapping</u> and take  $\rho=R$ , since, as shown by numerical experiments, this value of  $\rho$  is then <u>quasi-optimal</u>.

Remark 4.4. : It follows from [6] (see also [14]) that if p  $\ge$  2 (or for the finite dimensional problems approximating (4.1)) we have, for R<sub>Z</sub> replaced by I<sub>d</sub> and  $\rho$   $\in$  ]0,2R[,the following convergence results for algorithm (4.13)-(4.17):

$$\lim_{n \to +\infty} \{u^n, \underline{F}^n\} = \{\underline{u}, \underline{\nabla}u\} \quad \underline{\text{strongly in}} \ V \times H,$$

$$\lim_{n \to +\infty} \lambda^n = \left| \mathbf{v} \right|^{p-2} \mathbf{v} = \underbrace{\mathbf{weakly in}}_{\mathbf{h}^*} \mathbf{h}^*.$$

where u is the solution of (4.1).

Remark 4.5.: It is interesting to further analyse the structure of subproblems (4.15) and (4.16) which appear at each full step of the Uzawa algorithm used for the solution of our model problem (formulated as the equivalent saddle-point problem (4.10)). First, (4.15) in which

the variable is G, does not involve spatial derivatives of G; if a convenient discretization of H is used, it reduces (4.15) to a family of independent algebraic pointwise problems of the following type:

$$(4.18) \qquad \underset{G \in \mathbb{IR}^2}{\text{Min}} \left\{ \frac{1}{p} \left| \mathcal{G} \right|^p + \frac{R}{2} \left| \mathcal{G} - \nabla u_{k-1}^n \right|^2 - \lambda^n \cdot \mathcal{G} \right\}.$$

Solving problems like (4.18) is quite easy since  $|F_{k}^{n}|$  is the solution of the one variable minimization problem

$$\underset{z \in \mathbb{IR}_{\perp}}{\text{Min}} \left\{ \frac{1}{p} z^{p} + \frac{R}{2} z^{2} - \left| R \nabla u_{k-1}^{n} + \lambda^{n} \right| z \right\} .$$

Solving (4.19) by Newton's method is trivial ; then we obtain finally  $\mathbb{F}^n_k$  from  $|\mathbb{F}^n_k|$  by

$$F_{\sim k}^{n} = 0$$
 if  $R\nabla u_{k-1}^{n} + \lambda^{n} = 0$ ,

and in general

$$\mathbf{F}_{\mathbf{k}}^{n} = \left| \mathbf{F}_{\mathbf{k}}^{n} \right| \frac{(\mathbf{R} \nabla \mathbf{u}_{\mathbf{k}-1}^{n} + \lambda^{n})}{\left| \mathbf{R} \nabla \mathbf{u}_{\mathbf{k}-1}^{n} + \lambda^{n} \right|} .$$

On the other hand, (4.16) is a global quadratic minimization problem given by

(4.20) 
$$\min_{\mathbf{v} \in \mathbf{V}} \left\{ \frac{\mathbf{R}}{2} \int_{\Omega} \left| \nabla \mathbf{v} - \mathbf{F}_{\mathbf{k}}^{\mathbf{n}} \right|^{2} d\mathbf{x} + \int_{\Omega} \lambda^{\mathbf{n}} \cdot \nabla \mathbf{v} d\mathbf{x} - \int_{\Omega} \mathbf{f} \mathbf{v} d\mathbf{x} - \int_{\Gamma_{\mathbf{Q}}} \mathbf{g} \mathbf{v} d\Gamma \right\} ;$$

problem (4.20) is in fact equivalent to the following <u>linear</u> variational problem

$$\begin{cases} \frac{\text{Find}}{n} \, u_k^n \in V & \underline{\text{such that}} \\ R \int_{\Omega} \, \nabla u_k^n . \nabla v dx = \int_{\Omega} (R F_k^n - \lambda^n) . \nabla v dx + \int_{\Omega} f v dx + \int_{\Gamma_2} g v d\Gamma & \forall v \in V ; \end{cases}$$

we observe that  $\forall k$ ,n problems (4.21) are associated to the bilinear form  $\{v,w\} \to \int_{\Omega} \nabla v \cdot \nabla w \ dx$ .

Therefore we have achieved a decomposition of our model problem into a sequence of pointwise nonlinear algebraic problems which can be solved easily by Newton's type methods in  $\mathbb R$  and of elliptic linear problems, associated to the <u>same</u> bilinear form and whose finite dimensional approximations can be solved by either direct methods (such as Cholesky's) or efficient iterative methods.

Remark 4.6.: Although not critical, the choice of good values for R is complicated; theoretically the speed of convergence of algorithm (4.13)-(4.17) increases with R but the efficiency of the block relaxation algorithm (4.14)-(4.16) deteriorates as R increases (see [6] for more details).

# 5. Application to Finite Elasticity

# 5.1. Generalities

The application of augmented lagrangian techniques to the solution of equilibrium problems in <a href="Finite Elasticity">Finite Elasticity</a> encounters three types of difficulties:

- (i) The choice of reasonable constitutive laws;
- (ii) The choice of a correct functional framework for the problem decomposition (there is no true convexity in hyper elasticity); (iii) The derivation of adequate iterative methods for the pointwise solution of the algebraic problems appearing after decomposition.

Since it corresponds to our more recent numerical results, we will concentrate herein on the case of <u>compressible hyperelastic</u> bodies. The other case, concerning <u>incompressible</u> bodies, has already been extensively described in [9],[10] and [11] and is quite similar.

# 5.2. Formulation of equilibrium problems in compressible hyperelasticity.

The problem that we consider consists in the determination of the final equilibrium position of an hyperelastic compressible body subjected to large deformations through the application of given external loads and imposed boundary displacements. We label any particle  $\underline{x}$  of the body by its position in a stress free reference configuration (lagrangian coordinates) and we relate both  $\underline{x}$  and the displacement  $\underline{u}(\underline{x})$  to a fixed cartesian system. With these conventions, the interior of the body can be identified with an open set  $\Omega$  of  $\mathbb{R}^N$  (N=2 or 3). The body is subjected to body forces of intensity  $\underline{f}$  per unit volume in the reference configuration and to surface tractions  $\underline{g}$ , measured per unit area in the reference configuration, prescribed on a portion  $\Gamma_2$  of the boundary  $\Gamma$  of  $\Omega$ . Both  $\underline{f}$  and  $\underline{g}$  might depend on the displacement field  $\underline{u}$ . This displacement field takes on prescribed values  $\underline{u}_0$  on a portion  $\Gamma_1$  of  $\Gamma$  and we have :

$$\Gamma = \Gamma_1 \cup \Gamma_2$$
,  $\mathring{\Gamma}_1 \cap \mathring{\Gamma}_2 = \emptyset$ .

Writting the laws of force and moment balance in lagrangian coordinates, and for a given law of hyperelastic type on  $\Omega$ , we can characterize formally the equilibrium positions of the considered body as the solution of the following system :

(5.1) 
$$\begin{cases} -\nabla \cdot T_{R} = \int_{-\infty}^{\infty} \frac{\underline{i} n}{n} & \Omega , \\ T_{R} v = g & \underline{o} n & \Gamma_{2} \end{cases}$$

(balance of forces and moments) ;

(5.2) 
$$\underline{T}_{R} = \frac{\partial W}{\partial (\nabla u)} (\underline{x}, \underline{I} + \underline{\nabla} \underline{u}, \text{ adj} (\underline{I} + \underline{\nabla} \underline{u}), \text{ det} (\underline{I} + \underline{\nabla} \underline{u}))$$

(hyperelastic constitutive law) ;

(5.3) 
$$\det(I+\nabla u) \geq 0$$
 a.e. in  $\Omega$ ,

(orientation preservation) ;

$$(5.4) u = u \quad \underline{on} \quad \Gamma_1 .$$

In the above relations,  $T_R$  denotes the first <u>Piola-Kirchoff stress tensor</u> (whose mechanical interpretation is given in e.g. [17], [3], [12]),  $\nu$  denotes the <u>outward unit normal vector</u> in  $\Gamma_2$ , before deformation, and W the <u>elastic stored energy density</u>, per unit volume of the reference configuration. Typically, this stored energy density function W is of the following type

$$(5.5) W(x,F,G,\delta) = \mathcal{G}_1(x,F) + \mathcal{G}_2(x,F,G,\delta),$$

where  $\mathcal{G}_1$  is a regular convex real valued function defined on  $\Omega \times \mathbb{R}^{N^2}$  and where  $\mathcal{G}_2$ , from  $\Omega \times \mathbb{R}^{N^2} \times \mathbb{R}^N \times \mathbb{R}^N$  into  $\mathbb{R} \cup \{+\infty\}$  can be singular at  $\delta = 0$ . For example, for OGDEN's type materials, we have (cf. [4]):

(5.6) 
$$W(\underline{x}, \underline{F}, \underline{G}, \delta) = C_1 |\underline{F}|^2 + |C_2|\underline{G}|^2 + |C_3|^2 + |C_4|^2 + |C_$$

with  $C_1$ , i=1,2,3,4, nonnegative coefficients, and where, for a tensor X, |X| denotes the euclidian norm of X considered as an element of  $\mathbb{R}^{\mathbb{N}^2}$ .

For a constitutive law, such as (5.2), (5.5), we may formulate

the equilibrium system (5.1)-(5.4) as a variational problem as follows:

$$\underline{\text{Find}}\ \underline{\textbf{u}}\ \in\ \{\textbf{U}^{1,\textbf{S}}+\ \underline{\textbf{u}}_{\textbf{O}}\}\ ,\ \underline{\textbf{A}}\ \in\ (\textbf{L}^{\textbf{S}^{*}}(\Omega))^{N^{2}}\ \underline{\text{such that}}$$

(5.7) 
$$\delta = \det (I + \nabla u) \ge 0$$
 a.e. in  $\Omega$ ,

the notation  $adj(\tilde{F})$  denotes the adjugate of  $\tilde{F}$ , i.e. the <u>transpose of</u> the cofactor matrix. The usual notations are used for  $L^{S}(\Omega)$ ,  $L^{S^{*}}(\Omega)$  ( $s^{*} = \frac{S}{S-1}$ ) and the Sobolev space  $W^{1,S}(\Omega)$ ; we have

(5.10) 
$$U^{1,s} = \{ v | v \in (W^{1,s}(\Omega))^N, v = 0 \text{ on } \Gamma_1 \},$$

$$(5.11) U^{1,s} + \underset{\sim}{\mathbf{u}} = \{ \underbrace{\mathbf{v}} | \underbrace{\mathbf{v}} \in (\mathbf{W}^{1,s}(\Omega))^{N}, \underbrace{\mathbf{v}} = \underbrace{\mathbf{u}}_{\sim 0} \quad \underline{\text{on}} \quad \Gamma_{1} \}.$$

The exponent s is related to the energy density function W by continuity and coercivity properties. From a mechanical point of view the variational problem (5.7)-(5.9) is obtained from (5.1)-(5.4) by applying the virtual work principle for displacements v compatible with the boundary condition (5.4) (constraint (5.7) does not appear in the variational equations (5.8) where virtual displacement fields v possibly incompatible with (5.7) are allowed; however, for adequate W (such as (5.6), for example), smooth solutions of (5.8), (5.9) will satisfy (5.7)). Actually the variational formulation (5.7)-(5.9) is unusual in finite elasticity, where A is often eliminated between (5.8) and (5.9). However, formulation (5.7)-(5.9) is quite interesting since it is close from the variational formulation of equilibrium problems in incompressible hyperelasticity. Under that form, the augmented lagrangian decomposition described in Sec. 4, already introduced in [9] for incompressible hyperelasticity, can be easily generalized to compressible hyperelasticity.

# 5.3. An augmented lagrangian formulation of (5.7)-(5.9).

The extra variable needed for the decomposition of the equilibrium equations appears quite naturally to be the  $\frac{\text{deformation gradient}}{\text{matrix}}$ 

$$(5.12) F = I + \nabla u .$$

The augmented lagrangian  $\mathcal{Z}_{_{\mathrm{R}}}$  associated to our problem is then

$$\begin{cases} \mathcal{X}_{R}(\underline{y},\underline{H},\underline{\mu}) &= \int_{\Omega} \mathcal{G}_{1}(\underline{x},\underline{I} + \underline{y}\underline{y}) \, d\underline{x} + \int_{\Omega} \mathcal{G}_{2}(\underline{x},\underline{H},ad\underline{j}\underline{H},det\underline{H}) \, d\underline{x} + \\ + \frac{R}{2} \int_{\Omega} |\underline{I} + \underline{y}\underline{y} - \underline{H}|^{2} d\underline{x} + \int_{\Omega} \underline{\mu} \cdot (\underline{I} + \underline{y}\underline{y} - \underline{H}) \, d\underline{x} , \end{cases}$$

R being an arbitrary strictly positive constant. Now, as in Sec. 4, the variational system (5.7)-(5.9) of equilibrium equations can be written equivalently as the lagrangian system below:

$$(5.14) \qquad \frac{\operatorname{Find}}{\partial \mathbf{z}} \left\{ \underbrace{\mathbf{u}}, \underbrace{\mathbf{F}}, \underbrace{\lambda} \right\} \in \left( \mathbf{U}^{1}, \mathbf{s} + \underbrace{\mathbf{u}}_{0} \right) \times \mathbf{Y} \times \left( \mathbf{L}^{\mathbf{s}^{*}} (\Omega) \right)^{N^{2}} \xrightarrow{\text{such that}}$$

$$(5.14) \qquad \frac{\partial \mathbf{z}_{R}}{\partial \mathbf{u}} \left( \mathbf{u}, \underbrace{\mathbf{F}}, \underbrace{\lambda} \right) \cdot \underbrace{\mathbf{v}} = \int_{\Omega} \underbrace{\mathbf{f}} \cdot \underbrace{\mathbf{v}} \, d\mathbf{x} + \int_{\Gamma_{2}} \underbrace{\mathbf{g}} \cdot \underbrace{\mathbf{v}} \, d\Gamma \qquad \forall \underbrace{\mathbf{v}} \in \mathbf{U}^{1}, \mathbf{s} ,$$

$$(5.15) \qquad \frac{\partial \mathbf{z}_{R}}{\partial \mathbf{F}} \left( \underbrace{\mathbf{u}}, \underbrace{\mathbf{F}}, \underbrace{\lambda} \right) \cdot \underbrace{\mathbf{H}} = \mathbf{0} \qquad \forall \underbrace{\mathbf{H}} \in \left( \mathbf{L}^{\mathbf{S}} (\Omega) \right)^{N^{2}} ,$$

$$(5.16) \qquad \frac{\partial \mathcal{Z}_{R}}{\partial \tilde{\lambda}}(\tilde{u}, \tilde{F}, \tilde{\lambda}) \cdot \tilde{\mu} \equiv \int_{\Omega} (\tilde{I} + \tilde{\lambda}\tilde{u} - \tilde{F}) \cdot \tilde{\mu} \, dx = 0 \quad \forall \tilde{\mu} \in (L^{s^*}(\Omega))^{N^2}.$$

In the above relations, Y denotes the set of those elements H of (L  $^{\mathbf{S}}\left(\Omega\right)$  )  $^{N2}$  such that

det 
$$H \ge 0$$
 a.e. on  $\Omega$ .

5.4. Solution algorithm for the lagrangian system (5.14)-(5.16). We apply to the solution of (5.14)-(5.16) an algorithm, similar

to (4.13)-(4.17) of Sec. 4.3, and defined as follows:

$$(5.17) \qquad \{\hat{\chi}^{O}, \hat{u}^{-1}\} \in (L^{s^{*}}(\Omega))^{N^{2}} \times \{U^{1}, s_{u_{O}}\} \quad \underline{\text{is given}} ;$$

then, for  $n \ge 0$ ,  $u^{n-1}$  and  $\lambda^n$  being known, we compute  $\{u^n, v^n\}$  by block relaxation, i.e. by

$$(5.18) \qquad \underline{\text{setting }} \underbrace{u}_{O}^{n} = \underbrace{u}_{O}^{n-1},$$

and by computing sequentially  $u_k^n$  and  $F_k^n$  by solving

$$(5.19) \qquad \frac{\partial \mathcal{Z}_{R}}{\partial F}(\underline{u}_{k-1}^{n}, \underline{F}_{k}^{n}, \underline{\lambda}^{n}) \cdot \underline{H} = 0 \quad \forall \underline{H} \in (L^{S}(\Omega))^{N^{2}},$$

$$\begin{cases} \int_{\Omega} \frac{\partial \mathcal{Z}_{1}}{\partial (\underline{\nabla}\underline{u})} (\underline{x}, \underline{I} + \underline{\nabla}\underline{u}_{k}^{n}) + R(\underline{I} + \underline{\nabla}\underline{u}_{k}^{n} - \underline{F}_{k}^{n}) + \underline{\lambda}^{n} \} \cdot \underline{\nabla} v dx = \\ = \int_{\Omega} \underbrace{f \cdot \underline{v}}_{\Omega} dx + \int_{\Gamma_{2}} \underbrace{g \cdot \underline{v}}_{\Omega} d\Gamma, \quad \forall \underline{v} \in \underline{U}^{1}, \underline{s}, \quad \underline{u}_{k}^{n} \in \underline{U}^{1}, \underline{s} + \underline{u}_{0};$$

$$\underbrace{and}_{\Omega} \{\underline{u}^{n}, \underline{F}^{n}\}_{N}^{n} \underline{known}, \quad \underline{\lambda}^{n} \underline{is} \underline{updated} \underline{by}$$

$$(5.21) \qquad \lambda^{n+1} = \lambda^{n} + \rho R_{\pi}(\underline{I} + \underline{\nabla}\underline{u}^{n} - \underline{F}^{n}), \quad \rho > 0.$$

(5.21)

In the numerical applications, since we are always working with finite dimensional approximations of  $(L^{S}(\Omega))^{N^{2}}$ , the Riesz mapping R is replaced by the identity mapping. The updating of  $\lambda^n$  by (5.21) is then straightforward and the whole algorithm above reduces the solution of the equilibrium equations in compressible hyperelasticity to a sequence of convex displacement problems (5.20) (quadratic if (5.6) holds) and local deformation gradient problems (5.19).

Since  $\mathcal{C}_1$  corresponds only to the convex part of the elastic energy function W, the displacement problem (5.20) corresponds formally to an unconstrained uniformly convex minimization problem, set linear space U<sup>1, s</sup>. Among all the solution methods existing for such problems, we have chosen a conjugate gradient method with preconditioning by incomplete Cholesky factorization (ICGG algorithm; see [21] ). The preconditioning matrix is taken symmetric, positive definite, sparse, and invariant during the iterative process. Its "inversion" will be therefore very cheap, even in the case of large three-dimensional finite element approximations of U<sup>1,s</sup>. Due to the convexity of  $\mathcal{G}_1$  in (5.20), and since the solution  $u_{k-1}^n$  at the previous step is usually a good approximation of  $u_k^n$ . The conjugate gradient algorithm will converge quite quickly. Nevertheless, a special attention must be paid to the choice of the preconditioning matrix, in order to avoid unnecessary oscillations in the iterative process (5.17) - (5.21).

# 5.5. Three-dimensional analysis of the deformation gradient local problems (5.19).

If  $(L^{s}(\Omega))^{N^2}$  is approximated by a space of piecewise functions, problem (5.19), which does not involve any spatial derivative of F,

reduces to a sequence of independent local problems. For R sufficiently large, one can prove (cf. [18]) that each local problem is equivalent to

(5.22) 
$$\min_{\substack{F \in Y_{10C} \\ \text{for } \\ \text{for } \\ \text{for } }} \{ \hat{y}_{2}(\underline{x}, \underline{F}, \text{adj}\underline{F}, \text{det}\underline{F}) + \frac{R}{2} |\underline{F} - \underline{I} - \underline{V} u_{k-1}^{n}|^{2} - \underline{\lambda}^{n} .\underline{F} \} ,$$

with

$$Y_{loc} = \{F \in \mathbb{R}^{N^2}, \det F \geq 0\}.$$

If, as it is generally the case,  $\mathcal{G}_2$  takes infinite values for non positive values of det F, then we can replace  $Y_{loc}$  by  $\mathbb{R}^{N^2}$ . Due to its small dimension this problem could have been solved, in principle, by standard minimization technique for multidimensional algebraic functions. But in fact, due to its local structure which involves F, its adjugate and its determinant, (5.22) can be reduced to a one dimensional minimization problem if N=2, or to a sequence of one dimensional convex minimization problems if N=3. From now on we restrict ourselves to the most difficult case N=3 (three dimensional structures).

The <u>decomposition</u> of the local minimization problem for N=3 is again based on <u>augmented lagrangian techniques</u>. For that purpose, we introduce three new variables  $f \in \mathbb{R}^{36}$ ,  $g \in \mathbb{R}^9$  and  $G \in \mathbb{R}^9$  which allow a simple expression of adj f and det f as functions of f and which are defined by

Table 5.1.

(5.24) 
$$f = T F (T given by Table 5.1),$$

(5.24) 
$$f = T F \left( T \text{ given by Table 5.1} \right),$$

$$\left( g_{j} = \frac{1}{2} \varepsilon_{i} f_{4j-4+i}^{2}, \right)$$

$$\left( \forall j=1,\ldots,9, i=1,\ldots,4, \varepsilon_{1} = -\varepsilon_{2} = -\varepsilon_{3} = \varepsilon_{4} = 1, \right)$$

$$(5.26)$$
 G = g.

With these new variables, it is easy to calculate

adj 
$$F = G^T$$
, det  $F = F.G/3$ .

Let us now introduce the following local augmented lagrangian

(5.27) 
$$\begin{cases} \mathcal{Z}_{\ell}(\{F,G\},\{f,g\},\{f,g\},\{z,t\}) = \mathcal{G}_{2}(x,F,G,F,G/3) + \frac{R}{2}|F-I-\nabla u_{k-1}^{n}|^{2} - \lambda^{n}.F + \frac{r}{2}\{|f-TF|^{2} + |g-G|^{2} - z.(f-TF)-t.(g-G), \end{cases}$$

r being a strictly positive constant. The local minimization problem (5.22) can then be decomposed into the equivalent system

the sets  $\mathbf{X}_{\varrho}$  ,  $\mathbf{Y}_{\varrho}$  ,  $\mathbf{Z}_{\varrho}$  being defined by

$$\mathbf{x}_{\ell} = \mathbf{R}^9 \times \mathbf{R}^9$$
,  $\mathbf{z}_{\ell} = \mathbf{R}^{36} \times \mathbf{R}^9$ , 
$$\mathbf{y}_{\ell} = \{\{\mathbf{f}, \mathbf{g}\} \in \mathbf{z}_{\ell}, \mathbf{g}_{\mathbf{i}} = \frac{1}{2} \epsilon_{\mathbf{i}} \mathbf{f}_{4\mathbf{i}+\mathbf{i}-4}^2\}$$
.

The solution of the local minimization problem (5.22) reduces, finally, to the iterative solution of its augmented lagrangian formulation (5.28) by an algorithm similar to (4.13)-(4.17) (cf. Sec. 4.3) (with  $\{F,G\},\{f,g\},\{z,t\}$  playing the role of u,F,  $\lambda$ , respectively). In this algorithm, two elementary subproblems appear

(5.30) 
$$\min_{\{f,g\} \in Y_0} \mathscr{L}_{\ell}(F_k^m, G_k^m, f,g,z^m, t^m) .$$

Problem (5.30) is similar to (5.29), but simpler. That's why we only detail below the solution of (5.29), referring to [18] for the solution of (5.30).

# 5.6. Solution of (5.29).

In this section, we suppose that the stored energy function W is of OGDEN's type and is given (cf.[4]) by

$$W(\underline{x}, \underline{F}, \underline{G}, \delta) = C_1 |\underline{F}|^2 + C_2 |\underline{G}|^2 + C_3 \delta^2 - C_4 \log \delta.$$

For this stored energy function, the solution of (5.29) is achieved by making the following change of variables

(5.31) 
$$U = F + \beta G, \quad V = F - \beta G,$$

with

(5.32) 
$$\alpha = R + 4r$$
,  $\beta = ((2C_2 + r)/(R+4r))^{1/2}$ 

Problem (5.29) is then transformed into:

(5.33) 
$$\min_{\{\underbrace{U},\underbrace{V}\} \in \mathbb{R}^{18}} \left\{ \underbrace{\frac{\alpha}{4}} (|\underbrace{U} - \underbrace{A}|^2 + |\underbrace{V} - \underbrace{B}|^2) + C_3 q^2 - C_4 \text{ Log } q \right\} ,$$

with

(5.34) 
$$q = F.G/3 = (|U|^2 - |V|^2)/12\beta$$

$$(5.35) \qquad \qquad \underset{\sim}{A} = \frac{1}{2} \left\{ R \left( \underset{\sim}{\nabla} \underline{u} + \underline{\underline{r}} \right) - \underset{\sim}{\lambda} + \underbrace{\underline{T}}^{t} \left( r \underline{f}_{k-1}^{m} - \underline{z}^{m} \right) + \left( r \underline{g}_{k-1}^{m} - \underline{t}^{m} \right) / \beta \right\} ,$$

(5.36) 
$$B = \frac{1}{2} \{ R(\nabla u + I) - \lambda + T^{t}(rf_{k-1}^{m} - z^{m}) - (rg_{k-1}^{m} - t^{m}) / \beta \}.$$

The solution of (5.33) is easy to compute and is given by

$$(5.37) \qquad \qquad U = A/(\frac{\alpha}{2} + p/6\beta), \quad V/(\frac{\alpha}{2} - p/6\beta).$$

where p is the unique solution in interval ]-3 $\alpha\beta$  ,3 $\alpha\beta$ [ of the single variable equation

(5.38) 
$$\left| \frac{A}{\alpha} \right|^2 / \left( \frac{\alpha}{2} + p/6\beta \right)^2 - \left| \frac{B}{\alpha} \right|^2 / \left( \frac{\alpha}{2} - p/6\beta \right)^2 - \frac{3\beta}{C_3} (p + \sqrt{p^2 + 8C_4}C_3) = 0$$

The numerical solution of (5.29) is thus simply obtained by

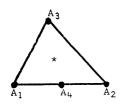
- (i) Solving (5.38) by (e.g.) a Newton's method,
- (ii) Computing {U,V} by (5.37),

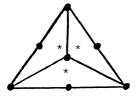
(iii) Computing  $\{F,G\}$ , from  $\{U,V\}$ , by solving (5.31), which is a trivial operation.

## 5.7. Axisymmetric numerical experiments.

The formulation of the equilibrium equations and the treatment of the deformation gradient local problems are given in [16] for the case of axisymmetric loadings of axisymmetric hyperelastic incompressible bodies. For the numerical solution of such problems, we choose here finite element approximations of the displacement space  $\mathbf{U}^{1,s}$  and of the deformation gradient space  $(\mathbf{L}^{s}(\Omega))^{s}$ , based on the 4 nodes asymmetric finite element developped by RUAS [25]. The element geometry is a triangle, the degrees of freedom for the displacements are their values at each vertex and at the midpoint of one side, the degrees of freedom for the deformation gradients are their values at the center of the triangles.

Assembling these elements 3 by 3 (as shown on Fig. 5.1) we obtain seven nodes symmetric finite superelements. The approximate displacements are taken continuous at element interfaces, the approximate deformation gradients are not since they are taken piecewise constant.





The asymmetric finite element: Symmetric assembly of 3 elements

- \* degrees of freedom in deformation gradients.
- degrees of freedom in displacements.

# Figure 5.1.

The numerical problem to be solved correspond then to the same lagrangian system (5.14)-(5.16), but set on the above finite element approximation of  $U^{1,s}$  and  $(L^{s}(\Omega))^{N^2}$ . Solution techniques remain unchanged compare to those described in the continuous case. The numerical example presented in this paragraph concerns the axial compression of an axisymmetric incompressible hyperelastic shaft whose shape is indica-

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ted below. For symmetry reasons, we restrict our domain  $\Omega$  to the upper meridian section of this shaft. The mesh before and after compression is represented on the figure below. We observe a surface discontinuity on the shaft after deformation, such a singularity is in complete agreement with the experimental studies and would be very difficult to obtain by usual numerical techniques.

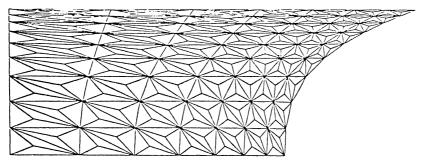


Figure 5.2.
Mesh before compression

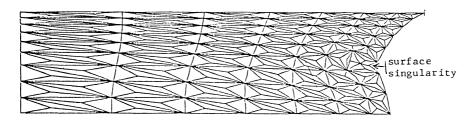
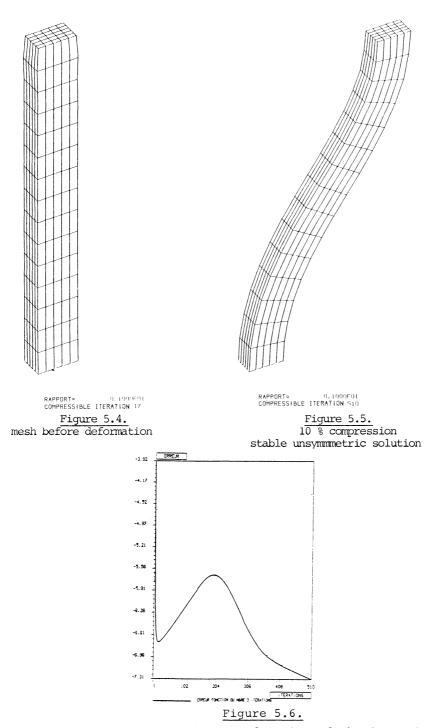


Figure 5.3.
30 % compression

Axisymmetric calculations for incompressible Mooney-Rivlin materials are discussed in Ref. [9] where comparisons with known analytical solutions are also presented.



Convergence rate as a function of the iteration number

# 5.8. Three dimensional numerical experiments.

The numerical example presented here illustrates the capability of the above numerical method for computing stable <u>postbuckling equilibrium positions</u> of hyperelastic bodies, even in three-dimensional configurations. The considered body is a 2×2×20 compressible elastic beam shortened to 90% of its initial length and subjected to a very small surface pressure on one of its faces. The stored energy function of the beam is supposed to be given by the function of (5.6) (i. e. we are dealing with an Ogden's material).

The displacement space is approximated by standard isoparametric 8 nodes hexahedral elements ( $\mathbf{Q}_1$  cubes), the approximate deformation gradients being constant on each element. Two solutions are then obtained by using the augmented lagrangian techniques of this paragraph: (i) an unstable symmetric solution with almost no horizontal displacements;

(ii) a stable unsymmetric solution with large horizontal displacements. The aspects of the beam before and after deformation is indicated on Figures 5.4 and 5.5, respectively. For symmetry reasons, we only consider the upper part of the beam.

It is particularly interesting here to monitor the convergence of the Uzawa algorithm. Measuring the convergence rate by  $\|\mathbf{I} + \nabla \mathbf{u}^n - \mathbf{F}^n\|_{0,2}$  at each iteration, we observe that this convergence indicator first decreases while the computed solution  $\mathbf{u}^n$  goes from zero to the unstable symmetric solution, then increases as  $\mathbf{u}^n$  automatically leaves the neighborhood of this symmetric solution, and finally decreases towards zero as  $\mathbf{u}^n$  approaches the final stable buckled solution (see Figure 5.6). This whole iterative process goes on completely automatically without any operator's action or incremental loading technique, by the simple execution of algorithm (5.17)-(5.21) with  $\mathbf{u}^0 = 0$ .

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