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NONLINEAR STRUCTURAL DYNAMICS VIA NEWTON AND QUASI-NEWTON METHODS *

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This paper is an attempt to compare Newton and quasi-Newton methods in nonlinear structural dynamics. After a review of the classical iterative methods, several quasi-Newton updates are presented and tested. Special attention is devoted to the solution of large sparse systems for which two original procedures are described: a substructure correction and a vectorial correction.

The numerical examples presented include the dynamic analyses of geometrical, material and combined nonlinearities. All the results are assorted with a complete discussion of the different methods used, of the convergence rates and of the associated computer costs.

From the present results, Newton's methods appear to exhibit the best convergence rates when an efficient computational strategy is adopted. Nevertheless computational costs for the solution of large systems can be reduced drastically by using convenient quasi-Newton updates.

1. Introduction

The best known method for solving large systems of nonlinear equations iteratively is Newton's method, sometimes modified so as to improve its computational efficiency. Davidon, for the minimization problem, and Broyden, for systems of equations, introduced new methods which, although iterative in nature, were quite unlike any other one in use at the time ([1]). This new class of algorithms has been called by the names quasi-Newton, variable metric, secant, update or modification methods.

In recent years there has been a proliferation of quasi-Newton methods applicable to the unconstrained minimization problem. The same is not true for solving nonlinear equations: According to [1], the only quasi-Newton method that has been seriously used to solve nonlinear equations is the one proposed by Broyden.

In the context of nonlinear structural analysis using the finite element method, advantage can be taken of the existence of a true functional for problems of finite elasticity, and of an incremental variational principle for problems involving also material nonlinearities: the resulting symmetric system of nonlinear equations can thus be solved using the quasi-Newton updates applicable to the minimization problem. The application of quasi-Newton methods to nonlinear structural equations has been suggested for the first time by Strang and Mathies [2] and the implementation of rank-two updates is discussed in [3,4,8].

Quasi-Newton methods seem to be particularly attractive to nonlinear dynamics analysis where the displacement increments are necessarily kept small in order to achieve a sufficient accuracy in the time-marching procedure [3,5].

In this paper it will be shown that various quasi-Newton updates are applicable to symmetric systems of equations, and that the relative simplicity of rank-one formulas makes them very attractive.

It will also be shown that in the context of nonlinear analysis using the finite element method, advantage can be taken of the sparse pattern of the structural matrices. Schubert [6] has proposed an algorithm which is of interest in the case of a sparse

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but non-symmetric system; a new update applicable to symmetric sparse systems is proposed here which takes into account the topology of the finite element mesh, and which can thus easily be implemented in a Gauss elimination scheme using the frontal concept.

Several problems of nonlinear dynamics in which geometric and material nonlinearities are simultaneously present will be considered, and their solution using various quasi-Newton updates will be compared to the solution using a Newton–Raphson strategy.

2. Newton–Raphson methods

Consider the problem of finding a solution to the system of n equations with n unknowns given by

$$r(q) = K(q)\,q - f(q) = 0\,, \tag{1}$$

where $K(q)$ is a $n \times n$ matrix, function of the unknowns q, and $f(q)$ the independent vector.

Newton's method for nonlinear equations can be derived by assuming that we have an approximation $\tilde{q}$ to q, and that in the neighbourhood of $\tilde{q}$ the linear mapping

$$r(q) = r(\tilde{q}) + \frac{\partial r(\tilde{q})}{\partial q}\,(q - \tilde{q}) \tag{2}$$

is a good approximation. A presumably better approximation can be obtained by equating eq. (2) to zero.

Thus, Newton's method takes an initial approximation q_0 to q, and attempts to improve it iteratively by

$$q_{k+1} = q_k - S^{-1}(q_k)\,r(q_k)\,, \tag{3}$$

with the definition of the tangent matrix

$$S = \partial r/\partial q\,. \tag{4}$$

In structural dynamics the vector $f(q)$ in eq. (1) is composed of two parts

$$f(q) = g_{\text{ext}} - M\ddot{q}\,, \tag{5}$$

where g_{ext} is the vector of time-dependent nodal loads, M the mass matrix and $\ddot{q}$ the acceleration vector. The main nonlinearities arise in general from material behavior or adaptation of the geometry, and are implicitly contained in the internal forces $K(q)\,q$ which result from the volume integration of the internal stresses σ

$$K(q)\,q = \int_v B^{\mathrm{T}}\sigma\,\mathrm{d}v\,. \tag{6}$$

The substitution of eq. (5) into eq. (2) yields

$$r(q) = r(\tilde{q}) + \left[K^{\mathrm{t}}(q) + M\frac{\partial\ddot{q}}{\partial q} - \frac{\partial g_{\text{ext}}}{\partial q}\right](q - \tilde{q})\,, \tag{7}$$

and shows that the tangent matrix is not only a function of the tangent stiffness matrix K^{t} but also of the time integration scheme used.

$$\dot{q}_{i+1} = \dot{q}_i + (1-\gamma)\,h\ddot{q}_i + \gamma h\ddot{q}_{i+1}\,, \tag{8}$$
$$q_{i+1} = q_i + h\dot{q}_i + (\tfrac{1}{2} - \beta)\,h^2\ddot{q}_i + \beta h^2\ddot{q}_{i+1}\,,$$

where the subscript i denotes the ith time-step, h the time-step and β, γ the Newmark's parameters [9], the tangent matrix becomes

$$S(q_k) = K^{\mathrm{t}}(q) + \frac{1}{\beta h^2}M + \frac{\partial g_{\text{ext}}}{\partial q}\,. \tag{9}$$

In the standard Newton–Raphson method of solution, successive corrections are then calculated assuming nullity of $r(q)$ in eq. (7).

The last term in eq. (9) is generally omitted to preserve the symmetry of the tangent matrix.

3. Quasi-Newton methods

3.1. Direct updates

The major expense in Newton's method is the calculation of $S(q_k)$ and its inversion.

In contrast, quasi-Newton methods consist to derive an approximation $\bar{S}$ to eq. (4) by evaluating $r(q)$ at two successive points q_k and q_{k+1}. Hence, if $\bar{S}$ is an approximation to S, it must satisfy eq. (2) rewritten in the form

$$\bar{S}d = g = r(q) - r(\tilde{q})\,, \tag{10}$$

where $d = q - \tilde{q}$.

Eq. (10) is called the quasi-Newton equation: all matrices satisfying eq. (10) are good candidates for $\bar{S}$. The simplest relation between S and $\bar{S}$ that satisfies eq. (10) is the single-rank update

$$\bar{S} = S + \frac{(g - Sd)\, u^{\mathrm{T}}}{u^{\mathrm{T}} d}, \tag{11}$$

for arbitrary u with $u^{\mathrm{T}} d \neq 0$.

Quasi-Newton iteration consists thus, given arbitrary q_0 and S_0, to calculate a new direction by eq. (3) and next, to generate a new matrix S_{k+1}:

$$d_k = -S_k^{-1} r_k\,, \tag{12}$$

$$S_{k+1} = S_k + \frac{(g_k - S_k d_k)\, u_k^{\mathrm{T}}}{u_k^{\mathrm{T}} d_k}\,, \tag{13}$$

where for simplicity all the indexed matrices S_k stand for the approximation matrix $\bar{S}$.

Several rank-one updates are possible: Broyden [7] proposes $u = d$ and shows that in this way $\bar{S}$ is the "closest" to S when measuring the distance by the Frobenius norm ([1]). Note that Broyden's update is unsymmetric and hence does not preserve the eventual symmetry of S.

For symmetric system of equations, Davidon suggests to use the direction $u = g - Sd$. The new corrective matrix becomes

$$\bar{S}_{\mathrm{D}} = S + \frac{(g - Sd)\,(g - Sd)^{\mathrm{T}}}{(g - Sd)^{\mathrm{T}}\, d}, \tag{14}$$

which insures the symmetry of the successive S_k.

Rank-two formulas are often proposed, for instance the Powell symmetric Broyden update (PSB), the Brodlie update, etc. Several of them, in addition to preserving symmetry, have the property of generating positive matrices. Among them, the most widely used are the Davidon–Fletcher–Powell update (DFP):

$$\bar{S}_{\mathrm{DFP}} = \left(I - \frac{g d^{\mathrm{T}}}{g^{\mathrm{T}} d}\right) S \left(I - \frac{d g^{\mathrm{T}}}{g^{\mathrm{T}} d}\right) + \frac{g g^{\mathrm{T}}}{g^{\mathrm{T}} d}\,, \tag{15}$$

and the Broyden–Fletcher–Goldfarb–Shanno formula (BFGS)

$$\bar{S}_{\mathrm{BFGS}} = S + \frac{g g^{\mathrm{T}}}{g^{\mathrm{T}} d} - \frac{S d d^{\mathrm{T}} S}{d^{\mathrm{T}} S d}\,. \tag{16}$$

Both formulas satisfy the quasi-Newton equation (10). In the same manner as for eq. (13), the iterative procedure is obtained by setting in eqs. (15–16) $\bar{S} = S_{k+1}, S = S_k, g = g_k, d = d_k$.

3.2. Inverse updates

To solve the linear problem eq. (12) at least expense it is convenient to obtain directly from eq. (11) the new approximation to the inverse S^{-1}. This is possible using the property that

$$(A - \alpha u v^{\mathrm{T}})^{-1} = A^{-1} - \beta y z^{\mathrm{T}}\,, \tag{17}$$

with $y = A^{-1} u$, $z = A^{-\mathrm{T}} v$ and $\beta = \alpha(1 + \alpha v^{\mathrm{T}} A^{-1} u)^{-1}$. Thus, the general rank-one update (11) becomes

$$\bar{S}^{-1} = S^{-1} + \frac{(d - S^{-1} g)\, v^{\mathrm{T}}}{v^{\mathrm{T}} g}\,, \tag{18}$$

for an arbitrary vector with $v^{\mathrm{T}} g \neq 0$. Broyden's update is obtained when $v = S^{-\mathrm{T}} d$, and Davidon's symmetric update when $v = d - S^{-1} g$. All the rank-two updates may also be transformed in the same manner to obtain directly the inverse matrix S^{-1}, yielding

$$\bar{S}^{-1}_{\mathrm{DFP}} = S^{-1} + \frac{d d^{\mathrm{T}}}{d^{\mathrm{T}} g} - \frac{S^{-1} g g^{\mathrm{T}} S^{-1}}{g^{\mathrm{T}} S^{-1} g} \tag{19}$$

and

$$\bar{S}^{-1}_{\mathrm{BFGS}} = \left(I - \frac{d g^{\mathrm{T}}}{g^{\mathrm{T}} d}\right) S^{-1} \left(I - \frac{g d^{\mathrm{T}}}{g^{\mathrm{T}} d}\right) + \frac{d d^{\mathrm{T}}}{g^{\mathrm{T}} d}\,. \tag{20}$$

It is useful to note that DFP and BFGS updates are related by the transformation

$$d \leftrightarrow g\,; \qquad \bar{S} \leftrightarrow \bar{S}^{-1}\,,$$

(see eqs. (15–20) and (16–19)); these updates are called "dual" or "complementary" updates ([1]).

3.3. Line search

In order to improve the convergence rate, the optimal step length σ_k can be evaluated such as to cancel the projection of the residual vector

$$\sigma = d_k^{\mathrm{T}} r(q_k + \sigma_k d_k) = 0\,, \tag{21}$$

and then

$$q_{k+1} = q_k + \Delta q_k$$

with

$$\Delta q_k = \sigma_k d_k\,. \tag{22}$$

This is an expensive operation since it may involve numerous evaluations of the residual vector to achieve great accuracy. One may expect, however, that the more accurate the line search is, the better is the chance of achieving convergence in a minimum number of iterations. In ref. [3], authors claim that satisfactory rate of convergence are provided when

$$|\boldsymbol{d}_k^{\mathrm{T}}\boldsymbol{r}(\boldsymbol{q}_k)| \geqslant 0.5\ |\boldsymbol{d}_k^{\mathrm{T}}\boldsymbol{r}(\boldsymbol{q}_k + \boldsymbol{d}_k)|\ . \tag{23}$$

This has been confirmed by the numerical experiments described in the present paper. When eq. (23) is not satisfied, successive linear interpolations are performed in order to obtain the optimal length σ_k such that

$$|\boldsymbol{d}_k^{\mathrm{T}}\boldsymbol{r}(\boldsymbol{q}_k)| \geqslant 0.5\ |\boldsymbol{d}_k^{\mathrm{T}}\boldsymbol{r}(\boldsymbol{q}_k + \sigma_k\boldsymbol{d}_k)|. \tag{24}$$

4. Quasi-Newton updates for sparse symmetric matrices

In many large systems of nonlinear equations, such as those resulting form a finite element discretization of nonlinear problems, most of the elements of the tangent matrix $\boldsymbol{S}$ are known to be zero owing to the topology of the finite element mesh. Obviously all the updates reviewed before do not yield sparse matrices. Schubert [6] proposed a variant of Broyden's unsymmetric update in which $\boldsymbol{S}_{k+1}$ is forced to have the same sparse pattern as $\boldsymbol{S}$. We expect, however, that for symmetric systems the best behavior would be obtained with a symmetric correction. This requires a simple modification of symmetric updates which will now be described.

4.1. Recursive procedure for substructure correction

Assume that in a finite element context a frontal method of solution is used, and that substructuring is adopted to perform block elimination. The tangent matrix $\boldsymbol{S}$ may then be split into a sum of N substructure contributions $\boldsymbol{S}_i$

$$\boldsymbol{S} = \sum_{i=1}^{N} \boldsymbol{L}_i^{\mathrm{T}}\boldsymbol{S}_i\boldsymbol{L}_i\ , \tag{25}$$

where $\boldsymbol{L}_i$ are incidence matrices.

Consider the problem of applying any rank-one symmetric correction of type

$$\bar{\boldsymbol{S}} = \boldsymbol{S} + \alpha\boldsymbol{c}\boldsymbol{c}^{\mathrm{T}}\ . \tag{26}$$

Any vector $\boldsymbol{c}$ can be decomposed into a sum of substructure contributions in the form

$$\boldsymbol{c} = \sum_{i=1}^{N} \boldsymbol{L}_i^{\mathrm{T}}\boldsymbol{c}_i\ . \tag{27}$$

This suggests a symmetric updating formula in which each block $\boldsymbol{S}_i$ is subjected to its own correction

$$\bar{\boldsymbol{S}} = \boldsymbol{S} + \sum_{i=1}^{N} \alpha_i\boldsymbol{L}_i^{\mathrm{T}}c_ic_i^{\mathrm{T}}\boldsymbol{L}_i\ , \tag{28}$$

and preserves thus the sparse pattern of the matrix. The coefficients α_i are not independent, since they must be chosen in order to satisfy eq. (10). For instance for $\boldsymbol{c} = \boldsymbol{g} - \boldsymbol{S}\Delta\boldsymbol{q}$ (Davidon's update), the coefficients are

$$\alpha_i = [\boldsymbol{c}_i^{\mathrm{T}}\boldsymbol{L}_i\Delta\boldsymbol{q}]^{-1}\ . \tag{29}$$

Rank-two formulas such as DFP may easily be transformed in the same manner to preserve the sparse pattern of the matrix. When the well-known substructuring technique is adopted to solve a system of equations, a Gauss elimination is made by block (substructure). Thus, the triangular matrix obtained has the same block pattern as the initial matrix. This characteristic allows to think of a special procedure to perform the correction directly on the triangular matrix instead of the initial matrix $\boldsymbol{S}$. In fact, consider first the problem of applying a rank-one correction $\alpha_i\boldsymbol{c}_i\boldsymbol{c}_i^{\mathrm{T}}$ to a given substructure of a symmetric matrix $\boldsymbol{S}_i$. At the substructure level i one has to solve a system which can be partitioned in the form

$$\begin{bmatrix} \boldsymbol{S}_{\mathrm{rr}} + \alpha_i\boldsymbol{c}_{\mathrm{r}}\boldsymbol{c}_{\mathrm{r}}^{\mathrm{T}} & \boldsymbol{S}_{\mathrm{rc}} + \alpha_i\boldsymbol{c}_{\mathrm{r}}\boldsymbol{c}_{\mathrm{c}}^{\mathrm{T}} \\ \boldsymbol{S}_{\mathrm{cr}} + \alpha_i\boldsymbol{c}_{\mathrm{c}}\boldsymbol{c}_{\mathrm{r}}^{\mathrm{T}} & \boldsymbol{S}_{\mathrm{cc}} + \alpha_i\boldsymbol{c}_{\mathrm{c}}\boldsymbol{c}_{\mathrm{c}}^{\mathrm{T}} \end{bmatrix} \begin{bmatrix} \Delta\boldsymbol{q}_{\mathrm{r}} \\ \Delta\boldsymbol{q}_{\mathrm{c}} \end{bmatrix} = \begin{bmatrix} -\boldsymbol{r}_{\mathrm{r}} \\ -\boldsymbol{r}_{\mathrm{c}} \end{bmatrix}, \tag{30}$$

where the indices r and c apply respectively to retained and condensed degrees of freedom.

In order to solve eq. (30), Gauss elimination is performed on the $\Delta\boldsymbol{q}_{\mathrm{c}}$, giving

$$\Delta\boldsymbol{q}_{\mathrm{c}} = \bar{\boldsymbol{S}}_{\mathrm{cc}}^{-1}[-\boldsymbol{r}_{\mathrm{c}} - \bar{\boldsymbol{S}}_{\mathrm{cr}}\boldsymbol{q}_{\mathrm{r}}]\ ,$$

and leads to

$$(\bar{\boldsymbol{S}}_{\mathrm{rr}} - \bar{\boldsymbol{S}}_{\mathrm{rc}}\bar{\boldsymbol{S}}_{\mathrm{cc}}^{-1}\bar{\boldsymbol{S}}_{\mathrm{cr}})\ \Delta\boldsymbol{q}_{\mathrm{r}} = -\boldsymbol{r}_{\mathrm{r}} + \bar{\boldsymbol{S}}_{\mathrm{cc}}^{-1}\boldsymbol{r}_{\mathrm{c}}\ ,$$

where the transformed matrices are

$$\text{(a)}\ \bar{S}_{cc}^{-1} = [S_{cc} + \alpha_i c_c c_c^T]^{-1} = S_{cc}^{-1} - \mu_i y_c y_c^T\ , \quad (31)$$

where

$$y_c = S_{cc}^{-1} c_c\ ,$$

and

$$\mu_i = \alpha_i/(1 + \alpha_i c_c^T y_c) \quad (32)$$

$$\text{(b)}\ \bar{S}_{cc}^{-1}\bar{S}_{cr} = [S_{cc} + \alpha_i c_c^T c_c]^{-1} \times [S_{cr} + \alpha_i c_c c_r^T]\ ,$$

or by making use of eqs. (31) and (32)

$$\bar{S}_{cc}^{-1}\bar{S}_{cr} = S_{cc}^{-1} S_{cr} + \mu_i y_c x_r^T\ , \quad (33)$$

where

$$x_r = c_r - S_{rc} y_c\ , \quad (34)$$

$$\text{(c)}\ \bar{S}_{rr} - \bar{S}_{rc} S_{cc}^{-1} \bar{S}_{cr} = S_{rr} + \alpha_i c_r c_r^T - [S_{rc} + \alpha_i c_r c_c^T] + [S_{cc}^{-1} S_{cr} + \mu_i y_c x_r^T]\ .$$

If account is taken of eqs. (32) and (34) we get

$$\bar{S}_{rr} - \bar{S}_{rc}\bar{S}_{cc}^{-1}\bar{S}_{cr} = S_{rr} - S_{rc} S_{cc}^{-1} S_{cr} + \mu_i x_r x_r^T\ . \quad (35)$$

(d) The inverse matrix is obtained in a similar form

$$[\bar{S}_{rr} - \bar{S}_{rc}\bar{S}_{cc}^{-1}\bar{S}_{cr}]^{-1} = [S_{rr} - S_{rc} S_{cc}^{-1}]^{-1} + \eta_i z_r z_r^T, \quad (36)$$

by introducing the vector $z_r = [S_{rr} - S_{rc} S_{cc}^{-1} S_{cr}]^{-1} x_r$ and the coefficient $\eta_i = \mu_i/(1 + \mu_i x_r^T z_r)$.

A rank-two correction such as specified in eq. (19) or eq. (20) may be organized in two successive rank-one corrections made in sequence: the second correction is written

$$\bar{\bar{S}} = \bar{S} + \gamma v v^T\ ,$$

and is performed according to eqs. (31), (33), and (35), but using the already modified matrices. Both corrections can be applied in one pass, without involving an intermediate memorization of the matrices.

Eq. (35) shows also that the correction applied on a given substructure i propagates to subsequent substructures $i + 1, i + 2, ..., N$ and yields thus to a total of $N(N + 1)/2$ rank-one or rank-two corrections performed.

In conclusion, the recursive procedure consists, given an arbitrary q_0 and a sparse matrix S_0, to perform the block elimination of the system only once. Then the successive updates are directly performed on the triangular matrix using eqs. (33)–(36).

4.2. Recursive procedure for vectorial correction

Another way of performing the quasi-Newton update consists of applying the correction on the direction Δq instead of modifying the matrix S directly. In fact, using the inverse update as described by eq. (18), the kth update of S^{-1} can be written as

$$S_k^{-1} = S_0^{-1} + \sum_{i=1}^{k-1} \beta_i v_i v_i^T\ . \quad (37)$$

For instance, for Davidon's update, we have $v_i = \Delta q_i - S_i^{-1} g_i$ and $\beta_i = [(\Delta q_i - S_i^{-1} g_i)^T g_i]^{-1}$. If at each iteration the correction vector v_i and coefficient β_i are stored on auxiliary memory, the $(k + 1)$ th direction can be obtained from eq. (12) as

$$d_{k+1} = -(S_0^{-1} + \sum_{i=1}^{k-1} \beta_i v_i v_i^T)\, r(q_k)\ . \quad (38)$$

The new correction vector for Davidon's update is then

$$v_k = \Delta q_k - S_0 g_k - \sum_{i=1}^{k-1} \beta_i v_i v_i^T g_k\ . \quad (39)$$

If an initial sparse matrix S_0 is given, it may be triangularized and stored only once. The successive product $S_0^{-1} r(q_k) = d_{0k}$ needed in eqs. (38) and (39) may be performed solving the system of equation

$$S_0 d_{0k} = r(q_k)\ .$$

In this manner only the nonzero elements of S_0 after Gauss elimination, the vectors v_i and the coefficients β_i have to be stored. When the number of correction vectors becomes too large, the algorithm may be restarted with the initial matrix S_0^{-1}. This procedure is applied by Crisfield [4] using only one correction vector at each iteration.

5. Numerical applications

5.1. Stretched cable submitted to transverse load

In order to appreciate the computational efficiency of quasi-Newton iteration, a first problem exhibiting strong geometric non-linearities has been examined.

It consists of a cable of span L stretched with an initial tension σ_0 between horizontal supports, with no sag and no initial transverse load. The dynamic loading consists of a linearly increasing, uniformly distributed transverse load $p(t) = p_0 t$ while the mechanical data are its extensional rigidity EA_0 and its mass per unit length $\rho_0 A_0$ (fig. 1).

The dynamic behavior of the cable is displayed in fig. 2 by means of the vertical motion of the mid-span node.

A linear solution, based on string theory, exists and is also represented which shows that the problem is highly non linear.

The problem has been solved using a finite element model of two cubic elements per half-span, and integrated in time using Newmark's scheme ($\beta = \frac{1}{4}, \gamma = \frac{1}{2}$).

With the standard Newton–Raphson method, different step sizes have been used: $\Delta t = 1, 2, 4$ and 6×10^{-3} s. The smallest Δt gives a converged solution, but $\Delta t = 2 \times 10^{-3}$ s still gives a solution with almost no deterioration. The solutions $\Delta t = 4$ and 6×10^{-3} s exhibit strong numerical damping and period elongation. In each case, stiffness reevaluation has been performed at iterations 1 and 2, and then every 3 iterations of each time step, unless the error measure $\|r\| \, \|g_{ext}\|^{-1}$ falls under the threshold $\epsilon_k = 1 \times 10^{-1}$. Equilibrium iteration is stopped when the same error measure becomes less than $\epsilon_R = 1 \times 10^{-3}$. One notes a progressive increase in the mean number of iterations per step to achieve dynamic equilibrium from 3 iterations/step when $\Delta t = 1 \times 10^{-3}$ to 5 iterations/step when $\Delta t = 6 \times 10^{-3}$ (fig. 3).

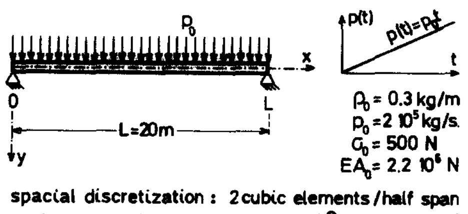

Fig. 1. Stretched cable submitted to transverse load.

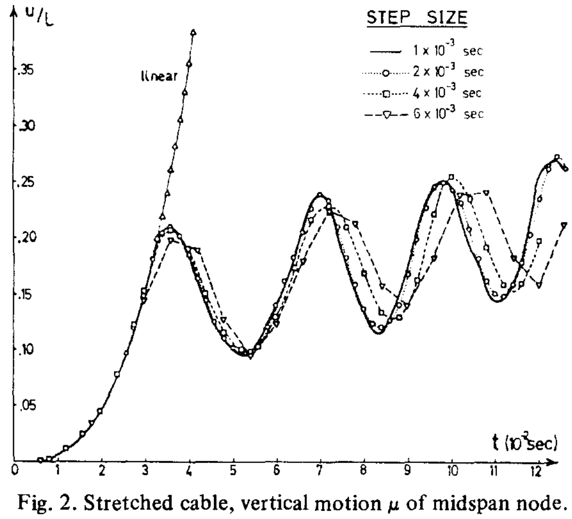

Fig. 2. Stretched cable, vertical motion μ of midspan node.

Quasi-Newton iteration with the BFGS update has been applied to the same problem with the step sizes $\Delta t = 1, 2$ and 4×10^{-3} s. Various strategies have been tried (see fig. 3), to measure the influence on the convergence of:

(i) the step size,

MODIFIED NEWTON ITERATION

STEP SIZE Δt (10^{-3} sec.)	MEAN N^{br} ITER./STEP
—— 1	3.0
---o--- 2	3.5
--□-- 4	4.6
—▽— 6	5.0

convergence parameters: $\epsilon_R = 10^{-3}$, $\epsilon_k = 10^{-1}$

no line search

stiffness updating (iterations) 1,2,5,8....

QUASI NEWTON ITERATION

convergence parameter : $\epsilon_R = 10^{-3}$

STEP SIZE Δt (10^{-3} sec.)	LINE SEARCH	STIFFNESS REEVALUATION (time steps)	MEAN N^{br} ITER./STEP
—— 1	yes	5	3.39
---o--- 2	yes	5	4.31
	yes	10	4.37
	yes	20	4.44
	yes	80	4.50
	no	10	4.93
--□-- 4	yes	20	5.68

Fig. 3. Stretched cable, influence of time step size.

(ii) the line search,

(iii) the frequency at which stiffness is reevaluated. The most instructive cases are those corresponding to $\Delta t = 2 \times 10^{-3}$ s. They show that periodic stiffness reevaluation has very limited influence on the convergence of the algorithm. The whole time history of the system can even be computed by performing quasi-Newton iteration without any direct evaluation of $\boldsymbol{K}^{t}$. They also show that roughly one more iteration per step is required: this results from the fact that the tangent iteration matrix at iteration i is determined after that the iteration has been actually made.

The line search has obviously a beneficial but limited effect on the method since a mean deterioration of 0.6 iteration/step is observed when skipping the line search. The best strategy would be to decide wether line search is desirable or not on the basis of the relative magnitude of the quantities $\boldsymbol{d}_i^{\mathrm{T}} \boldsymbol{r}(\boldsymbol{q}_i)$ and $\boldsymbol{d}_i^{\mathrm{T}} \boldsymbol{r}(\boldsymbol{q}_i + \boldsymbol{d}_i)$.

5.2. Simply-supported beam

The second example is the elastic–plastic dynamic analysis of a simply-supported beam to which a uniformly distributed pressure is suddenly applied The beam dimensions and material properties are described on fig. 4.

The elastic–plastic response is computed for an intensity of step pressure equal to 75% of the static collapse load. One quarter of the beam has been discretized with five cubic isoparametric elements ([11]) giving a total number of 42 d.o.f. Direct time integration has been performed with Newmark's scheme $\beta = 1/4, \gamma = 1/2$ in eq. (8) with a time step $\Delta t = 1.5 \times 10^{-4}$ s, which corresponds to 3/100 of the fundamental period of linear undamped vibration. Equilibrium iteration is stopped when $|\boldsymbol{r}|/(|\boldsymbol{g}_{\mathrm{ext}}| + |\boldsymbol{g}_{\mathrm{int}}|) \leqslant 10^{-3}$.

Fig. 5 shows the evolution of the displacement w at midspan for the linear and nonlinear solutions. No significant difference was observed between the Newton–Raphson and quasi-Newton solutions. The interest of the comparison lies in the number of iterations and CPU times required in both methods of solution.

The comparison is given by table 1 for the 30 first steps of the time history.

In the Newton–Raphson solution, the tangent stiffness is reevaluated at iterations 1, 2, 5 and 8 of each time step. When the material becomes linear, iteration is performed with the linear stiffness matrix. For quasi-Newton iteration, comparison is given between the following algorithms:

(a) The rank-one update of Davidon (eq. (14)) has been tested using successively the vectorial and substructure corrections as described in section 4.2. With the vectorial update, two possibilities have been investigated: starting the process at each time step either with the linear iteration matrix $\boldsymbol{S}_0$ (in which case only the evaluation of the linear stiffness matrix $\boldsymbol{K}_0$ is necessary) or with the tangent iteration matrix (which requires one matrix evaluation per time step). Stiffness reevaluation is an expensive operation, but leads always to a reduction of the number of evaluations of residual vectors. Due to the small size of this

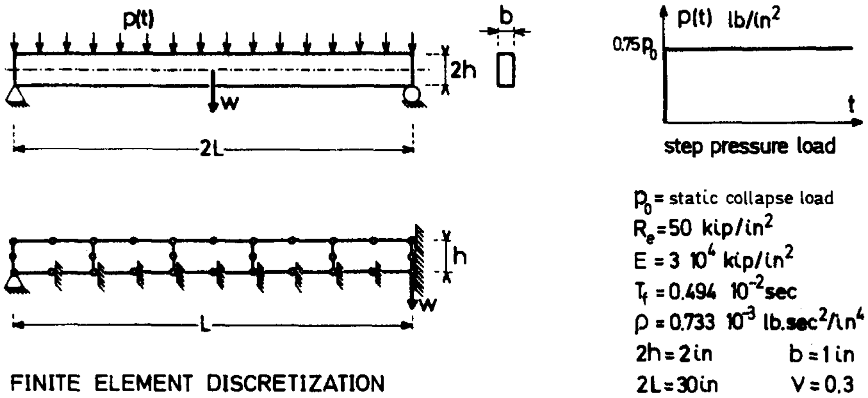

Fig. 4. Simply supported beam.

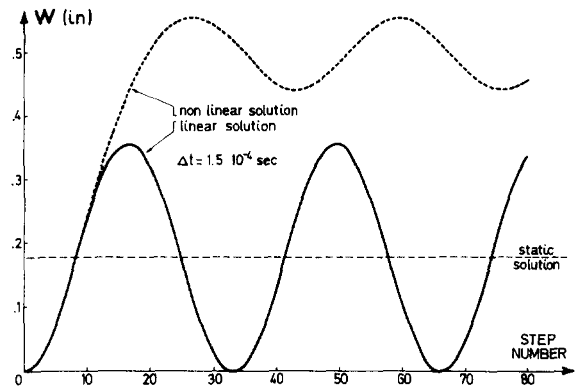

Fig. 5. Simply supported beam, displacement w at midspan node.

problem (42 d.o.f.) the difference of cost between a stiffness re-evaluation and a calculation of the residual vector is not sufficient to improve the total CPU time.

The rank-two update (BFGS, eq. (16)) has also been implemented with the substructure correction, and compared to Davidon's update. The recursive procedure described in 4.1 allows to start each time step with the approximate iteration matrix $\boldsymbol{S}$ evaluated before. However, if a large number of updates is carried out the matrix becomes ill-conditioned in this case, and a degradation in the convergence is then observed. With the substructure correction, the best solution corresponds always to starting each time step with the tangent iteration matrix. The rank-two correction does not bring a significant improvement in the convergence, and the cost of the double correction makes it noncompetitive with Davidon's update.

5.3. Spherical cap submitted to step pressure loading

The third example considered is that of a clamped spherical cap submitted to a sudden pressure loading, and where geometric and material nonlinearities are simultaneously present. Its geometric and material properties are summarized in fig. 6. This is a classical example taken from [10].

The structure is modelled with 8 axisymmetric cubic shell elements ([4]). The resulting F.E. model numbers 72 degrees of freedom. Only 3 Gauss points are used to integrate the constitutive law over the thickness: this relatively crude integration rule may be foreseen to generate oscillations in the numerical solution when plasticity develops. Time integration is performed with Newmark's scheme ($\beta = 1/4$, $\gamma = 1/2$) and a relatively large Δt of 1.5×10^{-5} s has been

Table 1
Simply supported beam – Comparison of the performances for different iteration methods

	Newton–Raphson	$\bar{S}_D$ update vectorial correction	$\bar{S}_D$ update vectorial correction (periodical stiffness re-evaluation)	$\bar{S}_D$ update substructure correction (periodical stiffness re-evaluation)	$\bar{S}_{BFGS}$ update substructure correction (periodical stiffness re-evaluation)
Number of iteration by step	2.9	4.73	2.8	2.67	2.67
Total number of stiffness re-evaluation	43	1	20	20	20
Total number of residual re-evaluation	87	172	127	120	124
Total number of Line search	–	–	13	10	14
C.P.U. time by iteration	2.58	1.87	2.59	2.94	3.12
Total numbee of iterations (30 steps)	87	142	84	80	80
Total C.P.U. time (30 steps)	224.1	266.8	218.0	235.0	249.6

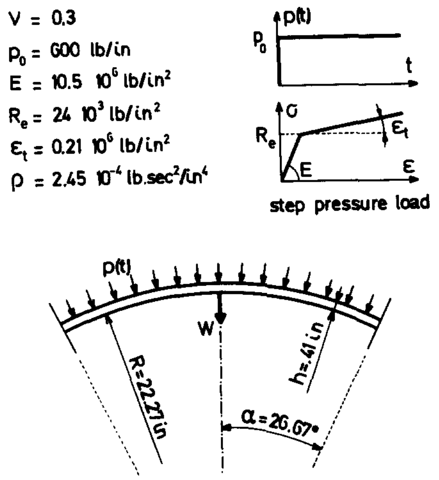

Fig. 6. Spherical cap submitted to step pressure loading.

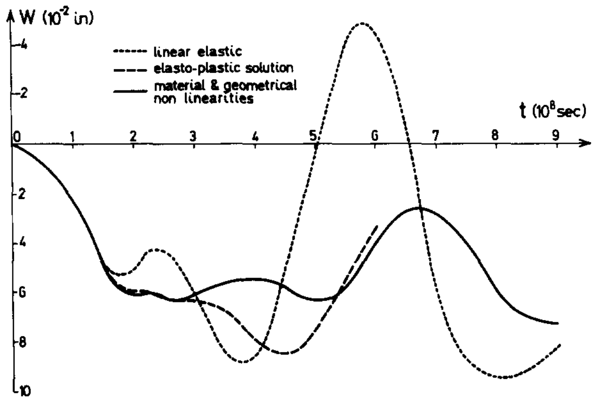

Fig. 7. Spherical cap, displacement w at midspan node.

adopted. Equilibrium iteration is stopped when

$$|r|/(g_{\text{ext}}| + |g_{\text{int}}|) \leqslant 10^{-3} .$$

Fig. 7 displays the time history of the axial displacement at the apex for the following solutions:

(i) linear elastic,

(ii) elastic-plastic material, geometrically linear,

(iii) material and geometrical non linearities simultaneously present.

Very little difference is observed in the numerical results with different methods of solution. For this example also, the only interest of the comparison lies in computer times and numbers of iterations to obtain the solution.

Again, to solve this problem, the comparison has been made between the Newton–Raphson iteration, and the quasi-Newton method using successively the Davidon and BFGS updates. The performances obtained to integrate the first 17 steps have been summarized in table 2.

The Newton–Raphson solution corresponds to a strategy in which stiffness is reevaluated at iterations

Table 2
Sperical Cap – Comparison of the performances for different iteration methods

	Newton–Raphson	$\mathcal{S}_D$ update vectorial correction (Line search)	$\mathcal{S}_D$ update vectorial correction	$\mathcal{S}_D$ update Substructure correction (periodical stiffness re-evaluation)	$\mathcal{S}_{BFGS}$ update Substructure correction (periodical stiffness re-evaluation)	$\mathcal{S}_{BFGS}$ update Substructure correction (Line Search)
Number of iteration by step	3.35	4.88	5.0	4.05	3.29	6.0
Total number of stiffness re-evaluation	40	1	1	17	17	1
Total number of residual re-evaluation	57	111	102	86	73	135
Total number of Line Search	–	11	–	–	–	16
C.P.U. time by iteration	5.40	2.97	2.75	4.2	4.83	3.6
Total number of iterations	57	83	85	69	56	102
Total C.P.U. time	308.0	247.0	233.6	290.0	271.0	368.0

1, 2, 5 and 8 of each time step.

Davidon's update has been tested using successively the vectorial correction (starting from K_0 at each time step) and the substructure correction (starting from the tangent stiffness matrix at each time step). The best results were obtained with the vectorial correction without line search.

The last two columns correspond to the BFGS updates. One observes a significant increase in the number of iterations when the process is not restarted at each time step, due to the fact that the number of updates on S_0 becomes excessive.

In this problem involving 72 degrees of freedom, the difference of computer cost between the reevaluation of stiffness (with Gauss elimination) and the calculation of the residual vector becomes significant, and renders quasi-Newton iteration more competitive.

6. Conclusions

(a) The existence of various updates to solve nonlinear problems of structural analysis has been demonstrated, and their implementation for large sparse systems using either vectorial or substructure corrections has been discussed.

(b) In most cases, it is observed that a too large number of quasi-Newton updates may lead to an ill-conditioned iteration matrix. It is thus advised to restart periodically the iteration procedure either using the initial stiffness S_0, or by calculating the tangent matrix.

(c) As a corallary, the vectorial correction is better adapted since it allows for an easy restart with S_0 at each time step.

(d) The line search does not introduce a significance improvment in the convergence of quasi-Newton methods, and should be performed only in exceptional cases.

(e) The rank-two correction does not yield an important improvement of the convergence rate. Hence, the Davidon rank-one correction should be preferred due to its lower cost.

(f) Quasi-Newton methods converge almost always in a larger number of steps than an "optimized" modified Newton strategy. They become thus competitive only when the cost of stiffness reevaluation becomes significantly larger than that of the residual vector calculation. This superiority of quasi-Newton methods is thus increased with the number of degrees of freedom as can be seen from the comparison of examples 2 and 3 where the saving in CPU time raises from 3% to 24%.

(g) It is worthwhile pointing out the fact that convergence difficulties may appear in situations of plastic unloading as occuring in examples 2 and 3. They constitute thus a severe test to evaluate the computational adequacy of all the iteration strategies that may be devised in nonlinear dynamics. Quasi-Newton methods have found to be very successful to treat them adequately.

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