M 7/1*

QUASI-NEWTON ITERATION IN NON-LINEAR STRUCTURAL DYNAMICS

M. GERADIN, M. A. HOGGE

Laboratoire d'Aéronautique, Université de Liège, rue du Val Benoit 75, B-4000 Liège, Belgium

SUMMARY

In the context of non linear structural dynamics, implicit methods of solutions involving the tangent stiffness matrix K^t are often not competitive with explicit schemes, due to the cost of the numerous updates of the iteration matrix $S = K^t + \beta h^{-2} M$ which are generally required for a satisfactory rate of convergence.

In an attempt to reduce this cost, the application of quasi-Newton methods seems to be particularly attractive : the underlying idea is to use an approximation to the inverse iteration matrix in place of the true inverse. Starting with an initial inverse matrix S_o^{-1}, successive corrections to the displacement are obtained from the quasi-tangent equations $S_{i-1} d_i = r_i$ where r_i, the residual vector, represents the lack of equilibrium. The next iteration matrix is expressed as the sum of the previous one and a rank-two correction. The optimal correction of displacement $\Delta q_i = \sigma_i d_i$ results from a line search such as to cancel the component of the residual vector along the direction of progression i.e. $d_i^T r(q_i + \sigma_i d_i) = 0$.

The method is particularly well adapted to nonlinear dynamics where the displacement increments are necessarily kept small in order to achieve a sufficient accuracy in the time-marching procedure. A few rank-two corrections lead at each step to a proper evaluation of the iteration matrix ; they involve only the calculation and combination of load vectors. The cost for updating the iteration matrix can thus be maintained at a much lower level than in the standard Newton procedure. The procedure can even be started with the direct stiffness matrix, making thus the availability of tangent stiffness calculations not essential.

Special care is devoted to the critical steps of the formulation :

- efficient implementation of the rank-two correction in gaussian elimination using the frontal concept ;
- minimum accuracy to be achieved in the line search process;
- frequency at which a direct evaluation of K^t is desirable to maintain the convergence of the solution.

The method is discussed on a benchmark problem of structural dynamics exhibiting strong geometric nonlinearities and indications are given on its performances in comparison with the standard Newton method.

1. Newton-Raphson iteration in nonlinear structural dynamics

In nonlinear structural dynamics, the basic matrix equation to be solved after spatial discretization is

$$M\ddot{q} = g_{ext} - g_{int} \tag{1}$$

with prescribed initial displacements $q(o)$ and velocities $\dot{q}(o)$, and where g_{ext} and g_{int} denote the external and internal forces at time t. The main nonlinearities arise in general from material behavior or changes in the geometry, and are implicitly contained in the internal forces which result from the volume integration of the internal stresses

$$g_{int}(q) = \int_V B^T \sigma \, dV \tag{2}$$

When an implicit finite difference scheme is used to integrate eq.(1) in time, the approximation to $\ddot{q}$ at time t_n is of the form

$$\ddot{q}_n = \beta h^{-2} q_n + s\,(q_{n-1}, \ddot{q}_{n-1}, q_{n-2}, \ddot{q}_{n-2}, \dots) \tag{3}$$

where the coefficient β and the function s describing the dependence on past motion depend on the integration formula used.

After substitution of the time discretization (3) into eq.(1), the displacement q_n is governed by the nonlinear equation

$$r(q_n) = g_{ext} - g_{int} - \beta h^{-2} M q_n - Ms(q_{n-1}, \ddot{q}_{n-1}, \dots) = o \tag{4}$$

If an approximate solution q_n is known, then displacements and accelerations can be incremented in the form

$$q_n = \tilde{q}_n + \Delta q \quad , \quad \ddot{q}_n = \tilde{\ddot{q}}_n + \beta h^{-2} \Delta q \tag{5}$$

and a Taylor expansion of eq.(4) around q_n yields

$$r_n = \tilde{r}_n + \left(\frac{\partial r}{\partial q}\right)_{\tilde{q}_n} \Delta q + O\,(\Delta q^2) \tag{6}$$

with the definition of residual vector representing the lack of dynamic equilibrium

$$\tilde{r}_n = r(\tilde{q}_n) = g_{ext} - g_{int}(\tilde{q}_n) - M\,\tilde{\ddot{q}}_n \tag{7}$$

and that of the tangent iteration matrix

$$\left(\frac{\partial r}{\partial q}\right)_{\tilde{q}_n} = -\left[\beta h^{-2} M + \left(\frac{\partial g_{int}}{\partial q}\right)_{\tilde{q}_n}\right] = -(\beta h^{-2} M + K^t) = -\,S(\tilde{q}_n) \tag{8}$$

K^t denotes in eq.(8) the tangent stiffness matrix of the structure.

If the standard Newton-Raphson method of solution is used, successive corrections are calculated by limiting eq.(6) to its first order expansion and assuming nullity of r_n :

$$\Delta q = [\,S(\tilde{q}_n)]^{-1}\,\tilde{r}_n \tag{9}$$

The method can be generalized by assuming a correction displacement in the direction (9), but with a step length σ

$$q_n = \tilde{q}_n + \sigma \Delta q \quad . \tag{10}$$

The progression parameter σ is adjusted to its optimal value, defined so that the component of the residual vector in the search direction is cancelled :

$$\Delta q^T r(\tilde{q}_n + \sigma \Delta q) = o \tag{11}$$

Within one time step, successive corrections Δq^i are calculated through eqs.(7-11) until the residual vector is rendered arbitrarily small. The high cost of an implicit time step results mainly from the reevaluation of the iteration matrix eq.(8) and its Gauss elimination involved in eq.(9).

This can be overcome to some extent with the so-called modified Newton method by keeping constant the iteration matrix for a few iterations or even over a few time steps, in which case a progressive degradation of the convergence properties of the algorithm is observed due to the increasing influence of non linearities. In [1], some numerical applications are presented on which the influence of stiffness updating frequency is displayed.

The line search eq.(11) can also represent a significant cost if numerous evaluations of the residual vector are necessary. If the nonlinearities within a time step remain sufficiently mild the successive optimal step lengths will always remain close to unity : assuming $\sigma = 1.0$ can then lead to a significant saving of computational effort. Otherwise, a line search based on linear interpolation generally provides sufficient accuracy.

2. Principle of the quasi-Newton method

As it has been pointed out in the previous section, the costly part of an iteration in the standard Newton-Raphson method is the updating and Gauss elimination of the stiffness matrix. As already demonstrated by STRANG and MATTHIES [2], quasi-Newton iteration provides an efficient means for reducing this cost.

It lies on the observation that, to the first order, eq.(6) provides an equation to be satisfied by the iteration matrix at $q = \tilde{q}_n$:

$$\left(\frac{\partial r}{\partial q}\right)_{\tilde{q}_n} \Delta q = r_n - \tilde{r}_n + O(\Delta q^2) \quad . \tag{12}$$

If q_n^i denotes the ith estimate of q_n, and if S_n^i is the approximation of the iteration matrix to be used to calculate a correction Δq^i to q_n^i, eq.(12) is the basis for the following iteration scheme :

- calculate a new search direction from the quasi-tangent equation

$$d^i = [S_n^{i-1}]^{-1} \, r_n^i \tag{13}$$

- compute the optimal step length σ^i such that

$$r(q_n^i + \sigma^i d^i) = 0 \quad , \tag{14}$$

  and set

$$\Delta q^i = \sigma^i d^i \quad , \quad q_n^{i+1} = q_n^i + \Delta q^i \tag{15}$$

- evaluate the residual vector $r_n^{i+1} = r(q_n^{i+1})$, and construct a new approximation to the iteration matrix at q_n^i (the updating procedure using rank-two corrections will be discussed in the next section) in order to satisfy eq.(12) :

$$- S_n^i \, \Delta q_n^i = r_n^{i+1} - r_n^i \tag{16}$$

The main difference with the standard Newton-Raphson method comes thus from eq.(13) : the correction Δq^i is now evaluated with the tangent iteration matrix at q_n^{i-1}. This time lag with which the iteration matrix is updated can be expected to introduce some degradation in the convergence properties of the method ; this will be checked on the numerical application.

The implicit iteration scheme with equilibrium iteration based on eqs.(13-16) can be implemented as shown on fig.1. The following remarks should be made :

1. If the time integration procedure is performed with a sufficiently small step size as required for the accuracy of the solution, the mass matrix term will remain dominant in the iteration matrix $S = (\beta h^{-2}M + K^{t})$. Hence, quasi-Newton iteration is particularly well adapted to non linear dynamics where only slight corrections are brought to the iteration matrix at two successive iterations or time steps.

2. Flexibility has to be given to the user in the choice of an updating strategy. The facility has to be provided for a periodic reevaluation of the tangent iteration matrix, and line search should be performed only when necessary.

3. In account of to the lag that exists between stiffness updating and displacement corrections, the quasi-Newton correction of the iteration matrix has to be skipped at the very first iteration of each time step. This observation is consitent with the fact that for linear applications no matrix updating is necessary.

3. Quasi-Newton correction to the iteration matrix

The problem is that of constructing recursively iteration matrices starting from an initial matrix S_o, such that (for conciseness of the equations, time indices are dropped and lower indices are now used to denote iterations)

$$S_{i-1}d_i = r_i \qquad \text{and} \qquad S_i\ \Delta q_i = -\ g_i \tag{17}$$

with the definitions

$$\Delta q_i = \sigma_i d_i \qquad \text{and} \qquad g_i = r_{i+1} - r_i \tag{18}$$

Symmetry of the iteration matrix is preserved using the classical rank-two correction [3] :

$$S_i = S_{i-1} + \alpha r_i r_i^T + \beta g_i g_i^T \tag{19}$$

with the coefficients $\alpha = -\ (r_i^T d_i)^{-1}$ and $\beta = -\ (g_i^T\ \Delta q_i)^{-1}$. The inverse matrix can also be obtained from a similar correction

$$S_i^{-1} = S_{i-1}^{-1} + \alpha^{*} d_i d_i^T + \beta^{*}(S_{i-1}^{-1}g_i)\ (S_{i-1}^{-1}g_i)^T \tag{20}$$

with $\qquad \alpha^{*} = -\ \sigma_i (d_i^T g_i)^{-1}$ and $\beta^{*} = (g_i^T S_i^{-1} g_i)^{-1}$

As it is shown in [2], if the positive definiteness of the iteration matrix is assumed, the transformation (20) can also be recast in the form of a skew projection

$$S_i^{-1} = (I + v_i w_i^T)\ S_{i-1}^{-1}(I + w_i v_i^T) \tag{21}$$

with the projection vectors $v_i = \phi d_i$ and $w_i = g_i - \psi r_i$ and the coefficients $\phi = -\ (d_i^T g_i)^{-1}$ and $\psi = \{\ \sigma_i\ [\ 1 - d_i^T r_{i+1} (r_i^T S_{i-1}^{-1} r_i)^{-1}]\ \}^{1/2}$

In its basic form eq.(20), the quasi-Newton correction applies only to iteration matrices that fit into central core memory. It is thus not applicable to large systems arising in finite element applications.

The correction in product form eq.(21) does not need to be performed explicitly on the iteration matrix. The successive projection directions may be stored on auxiliary device, in which case the corrections are applied in sequence before and after performing the linear solution (13). However, a significant increase of cost is then observedwith the number of iterations, and periodic stiffness reevaluations are then necessary to reduce the cost of the solution.

The numerical applications performed so far with the algorithm indicate that the stability of quasi-Newton iteration is such that periodic reevaluations of the iteration matrix are often superfluous from a convergence standpoint. This observation motivates the development of an out-of-core method of solution in which rank-two corrections can easily be implemented, as discussed in the next section.

4. Implementation of the rank-two correction in a frontal solution algorithm

In a finite element context, the problem arises of performing the corrections (19) or (20) on large systems of equations, generally solved using either Choleski decomposition or Gauss elimination organized out-of-core .

Let us concentrate on the frontal method of solution, and consider first the case of applying a rank-one correction to a symmetric matrix S : one has thus to solve a new system

$$[S + \alpha u u^T]\ x = b$$

which can be split in the form

$$\begin{bmatrix} S_{RR} + \alpha u_R u_R^T & S_{RC} + \alpha u_R u_C^T \\ S_{CR} + \alpha u_C u_R^T & S_{CC} + \alpha u_C u_C^T \end{bmatrix} \begin{bmatrix} x_R \\ x_C \end{bmatrix} = \begin{bmatrix} b_R \\ b_C \end{bmatrix} \qquad (22)$$

where the indices R and C apply to retained and condensed degrees of freedom, respectively.

In order to solve eq.(22) using the frontal concept, the following transformed matrices (denoted by an asterisk) must be calculated successively :

(i) $$[S_{CC}^{-1}]^{*} = [S_{CC} + \alpha u_C u_C^T]^{-1} = S_{CC}^{-1} + \beta y_C y_C^T \qquad (23)$$

where $$y_C = S_{CC}^{-1} u_C \qquad (24)$$

and $$\beta = -\alpha\ (1 + \alpha u_C^T y_C)^{-1} \ . \qquad (25)$$

(ii) $$[S_{CC}^{-1} S_{CR}]^{*} = [S_{CC} + \alpha u_C u_C^T]^{-1} [S_{CR} + \alpha u_R u_R^T]$$

By making use of eq.(23) and eq.(25), we get

$$[S_{CC}^{-1} S_{CR}]^{*} = S_{CC}^{-1} S_{CR} - \beta y_C \bar{u}_R^T \qquad (26)$$

where $$\bar{u}_R = u_R - S_{RC} y_C \ . \qquad (27)$$

(iii) $$[\overline{S}_{RR}]^{*} = [S_{RR} - S_{RC} S_{CC}^{-1} S_{CR}]^{*}$$

$$= S_{RR} + \alpha u_R u_R^T - [S_{RC} + \alpha u_R u_C^T]\ [S_{CC}^{-1} S_{CR} - \beta y_C \bar{u}_R^T]$$

If account is taken of eq.(25) and eq.(27), we have

$$[\overline{S}_{RR}]^{*} = \overline{S}_{RR} - \beta \bar{u}_R \bar{u}_R^T \ . \qquad (28)$$

Introducing the vector $\bar{z}_R = \overline{S}_{RR}^{-1} \bar{u}_R$, and the coefficient $\eta = \beta(1 - \beta \bar{u}_R^T \bar{z}_R)^{-1}$, its inverse is written

$$[\overline{S}_{RR}^{-1}]^{*} = \overline{S}_{RR}^{-1} + \eta \bar{z}_R \bar{z}_R^T \ . \qquad (29)$$

When the frontal concept is used, eq.(23 to 29) are applied recursively to perform a rank-one correction on the Gauss elimination scheme of the initial matrix S.

The rank-two correction involved in eq.(19) can be organized in two successive rank-one corrections made in sequence : the second correction on the matrix is written

$$S^{**} = S^{*} + \gamma v v^T$$

and is performed according to eq.(23), (26) and (29), but using the already modified matrices $[S_{CC}^{-1}]^{*}$, $[S_{CC}^{-1} S_{CR}]^{*}$ and $[\bar{S}_{RR}]^{*}$:

(i) $$[S_{CC}^{-1}]^{**} = [S_{CC}^{-1}]^{*} + \delta\, w_C w_C^T \qquad (30)$$

with the vector $$w_C = [S_{CC}^{-1}]^{*}\, v_C \qquad (31)$$

and $$\delta = -\gamma (1 + \gamma v_C^T w_C)^{-1} \qquad (32)$$

(ii) $$[S_{CC}^{-1} S_{CR}]^{**} = [S_{CC}^{-1} S_{CR}]^{*} - \delta w_C \bar{v}_R^T \qquad (33)$$

with $$\bar{v}_R = v_R - S_{RC} w_C \qquad (34)$$

(iii) $$[\bar{S}_{RR}]^{**} = [\bar{S}_{RR}]^{*} - \delta \bar{v}_R \bar{v}_R^T \qquad (35)$$

Both corrections can be made in one pass, without involving an intermediate memorization of the matrices $[S_{CC}^{-1}]^{*}$ and $[S_{CC}^{-1} S_{CR}]^{*}$.

5. Numerical application

In order to appreciate the computational efficiency of quasi-Newton iteration a dynamic problem exhibiting strong geometric nonlinearities has been analyzed.

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

The dynamic behavior of the cable is displayed on the figure 2 by means of the vertical motion u of the midspan node $x = L/2$.

A linear solution, based on string theory, exists and is also represented which shows that the problem is highly nonlinear : the linear and nonlinear solutions differ rapidly, and there is a drastic change in the period of the system (from 0.9798 sec in the linear case, to about 0.04 sec in the nonlinear case).

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

With the standard Newton method [1], four different step sizes have been used : Δt = 1, 2, 4 and 6.10^{-3}sec. The smallest step size gives a converged solution, but $\Delta t = 2.10^{-3}$ sec still gives a solution with almost no deterioration. The solution with Δt= 4 and 6.10^{-3} sec 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 $\varepsilon_k = 1.10^{-1}$. Equilibrium iteration is stopped when the same error measure becomes less than $\varepsilon_R = 1.10^{-3}$. One notes a progressive increase in the mean number of iterations per step to achieve dynamic equilibrium from 3.0 iterations per step when $\Delta t = 1.10^{-3}$sec, to 5.0 iterations per step with $\Delta t = 6.10^{-3}$sec.

Quasi-Newton iteration has been implemented with the same time integrator and applied to the same problem with the step sizes Δt=1,2 and 4.10^{-3}sec. Various strategies have been tried, as shown on the figure, to measure the influence on the convergence of :

- the step size,
- the frequency at which stiffness is reevaluated,
- the line search.

The most instructive cases are those corresponding to $\Delta t = 2.10^{-3}$ sec. 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 the tangent iteration matrix. 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 the iteration has been actually made.

The line search has obviously a beneficial effect on the convergence of the method since a mean deterioration of 1.2 iteration/step is observed when skipping the line search. The best strategy would be to decide automatically whether line search is desirable or not, on the basis of the relative magnitude of the quantities $d_i^T r(q_i)$ and $d_i^T r(q_i+d_i)$.

6. Conclusions

The effectiveness of the quasi-Newton method to reduce the computational effort, and thus the cost of the implicit solution of nonlinear dynamic problems has been demonstrated. An updating scheme based on the frontal concept has been proposed, which renders the method applicable to large finite element problems requiring an out-of-core solution. Further applications of the method to problems of increasing size and complexity will be considered in order to confirm the present results.

References

[1] G. SANDER, M. GERADIN, C. NYSSEN, M. HOGGE, "Accuracy Versus Computational Efficiency in Non Linear Dynamics", FENOMECH 78, ISD, Universität Stuttgart, 1978.

[2] H. MATHIES and G. STRANG, "The Solution of Non Linear Finite Element Applications", To appear in Int. Jnl. Num. Meth. in Engng.

[3] D.G. LUENBERGER, "Introduction to Linear and Nonlinear Programming", ch.9, Addison-Wesly, Reading, Ma, 1973.

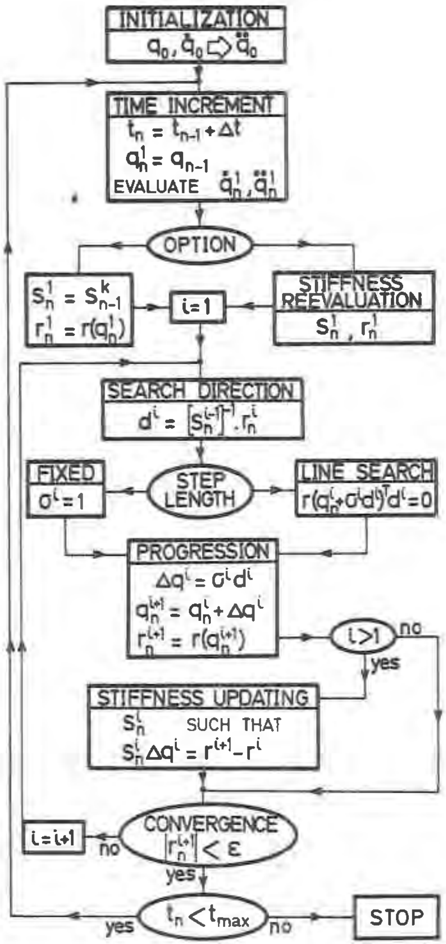
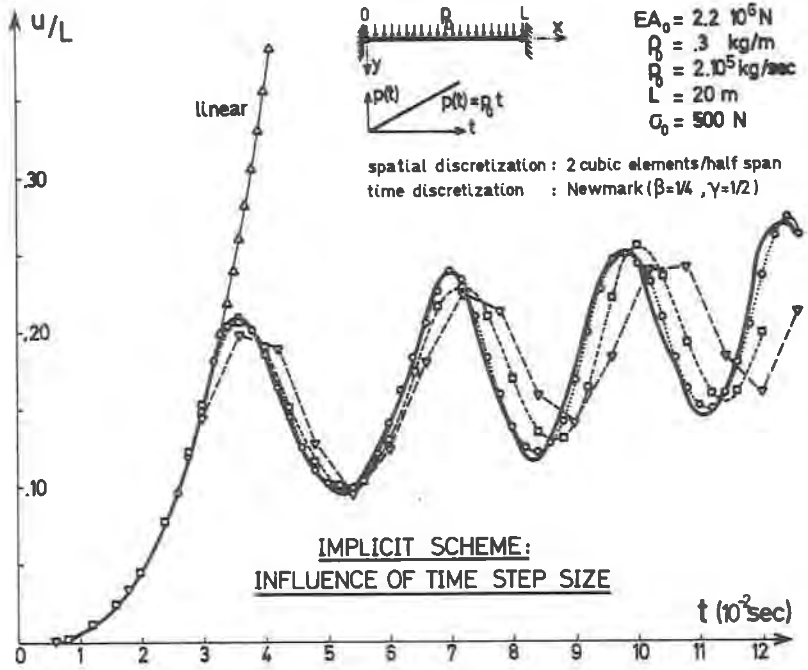


Fig. 1. IMPLICIT ITERATION SCHEME WITH QUASI-NEWTON UPDATING



MODIFIED NEWTON ITERATION

CONVERGENCE PARAMETERS: $\varepsilon_R = 10^{-3}, \varepsilon_k = 10^{-1}$

NO LINE SEARCH

STIFFNESS UPDATING (ITERATIONS) 1,2,5,8...

STEP SIZE Δt (10^{-3} sec)		MEAN Nbr ITER/STEP
———	1	3
····o····	2	3.5
---□---	4	4.6
—▽—	6	5

QUASI NEWTON ITERATION

CONVERGENCE PARAMETER: $\varepsilon_R = 10^{-3}$

STEP SIZE Δt (10^{-3} sec)		LINE SEARCH	STIFFNESS REEVALUATION (time steps)	MEAN Nbr 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. 2. STRETCHED CABLE SUBMITTED TO TRANSVERSE LOAD