AN EFFICIENCY ASSESSMENT OF SELECTED

UNCONSTRAINED MINIMIZATION TECHNIQUES

AS APPLIED TO NONLINEAR STRUCTURAL ANALYSES

by

Norman F. Knight, Jr.

Thesis submitted to the Graduate Faculty of the

Virginia Polytechnic Institute and State University

in partial fulfillment of the requirements for the degree of

MASTER OF SCIENCE

in

Engineering Mechanics

APPROVED:

M. P. Kamat, Chairman

F. J. Maher   C. W. Smith

J. E. Kaiser, Jr.

August, 1977

Blacksburg, Virginia

ACKNOWLEDGEMENTS

The author also wishes to express his deepest appreciation to his landlady,   , for her sincere interest, concern and friendship.

Beyond the scope of words, the author dedicates this thesis to his parents,   , without whose support, encouragement and prayers this thesis would not have been possible.

TABLE OF CONTENTS

TABLE OF CONTENTS (Continued)

LIST OF FIGURES

LIST OF TABLES

LIST OF TABLES (Continued)

1. INTRODUCTION

Within the realm of solid mechanics, all phenomena are intrinsically nonlinear. The mathematical complexities of nonlinear analysis have prolonged the formulation of nonlinear concepts which in turn imprison the understanding of such phenomena. Realistic engineering solutions may be derived from linear formulations in many instances, while others necessitate a nonlinear analysis. "We find that there are certain nonlinear concepts which at first appear complex, but which, when understood, are found to have universal applicability. In such cases, it is more profitable to master the concept in its non-linear aspect than to patch together strained linear concepts on the ground that linear concepts are inherently simpler" [1]. To this end, the reality of predicting nonlinear structural behavior was realized with the advent of the digital computer, the conception of the finite element technique for structural analysis [2] and the recognition of its equivalence with a minimization process [3,4]. The evolution of computerized structural analysis methods, as depicted by Felippa and Sharifi [5], is given in Table 1. The validation of given numerical methods of nonlinear analysis is often effectuated by comparison of its solution either with accessible experimental results or with results from previously established numerical methods. However, comparison with experimental results is preferable if possible for "experimental science does not receive truth from superior sciences; she is the mistress and the other sciences are her servants" [6].

1

Table 1. Evolution of Computerized Structural Analysis Methods
(From Reference 5; Used by Permission)

Year	Formulation Technology	Program Implementation Technology	Computer Technology	Generation
1950	Matrix transformation theory of structures		UNIVAC I	
	Force method	Equations set up by user		
		Standard matrix routines (assembly language)	IBM 704	1
1955	Stiffness method	Equations constructed by program	FORTRAN	
	2D elements	Higher order languages		
	Incremental nonlinear analysis	Block elimination solvers	Operating Systems	
1960	Structural optimization	Substructuring	IBM 7090	2
	3D elements	Iterative linear solvers		
	Variational formulation	Band solvers	CDC 6600	
	Complementary formulations	General-purpose linear codes	Direct-access mass storage	
	Incompatible displacement models	Sparse matrix techniques		
1965	Refined elements	Optimization packages	IBM 360	3
	Direct nonlinear analysis		Time sharing	
	Hybrid and mixed formulations	Design program networks & common data bases	Graphics	
	Finite difference energy models		Minicomputers	
	Space-time elements			
1970	Mathematical foundations and piecewise approximation theory	General-purpose nonlinear codes		4

0-6 years implementation lag

2-3 years lag in use of new features

2

The growth of computer assisted nonlinear structural analysis in recent years stems from an increased emphasis on realistic modelling and accurate response determination of critical structural components by private and governmental agencies. Coupled with this technological driving force are the aspirations for an economical, efficient and accurate solution procedure adaptive to existing computer hardware.

The most widely adopted method for present day structural analysis is the displacement formulation of the finite element method. In its most commonly used form for static analysis of structures, the method utilizes the principle of the minimum value of the total potential energy which can be stated as follows:

"A conservative holonomic system is in a configuration of

stable equilibrium if, and only if, the value of the

potential energy is a relative minimum" [7].

The minimization approach as applied to transient nonlinear structural analyses consists of minimizing a potential function which is associated with the structural characteristics of a system for an assumed relationship between displacements and time, such as the Newmark-Beta method [8].

Nonlinearities enter these potential functions through the functional representation of the structure's strain energy. The nonlinearities considered in this study arise from including the effects of either one or both of the following sources: (i) large rotations with small strains (geometric nonlinearity) and (ii) loading

and unloading in the inelastic range of a linear elastic material model with strain hardening in the inelastic range (material non-linearity).

For transient nonlinear analyses incorporating both geometric and material nonlinearities, the techniques most commonly utilized can be classified as follows: (i) explicit or implicit time integration schemes in conjunction with an incremental stiffness approach; and, (ii) explicit or implicit time integration schemes utilizing an explicit evaluation of the vector of internal nodal forces [10]. The method of the former category is not tailored for highly nonlinear problems unless one resorts to iteration at constant load to avoid large inaccuracies [10]. The solution effort of the method in the latter category is presumably minimal with an explicit time integration scheme and moderate with an implicit scheme.

It is well known that more often than not inertial problems such as those involving the elastic-plastic, large deformation response of structures are best solved by implicit techniques [10]. Since the computational effort within a load or time step is by no means small with an implicit scheme, the minimization algorithms are appealing and demand a rigorous evaluation of their effectiveness in solving nonlinear problems especially of the inertial category. It must be recognized that once the assumption of a displacement-time relation is made, the minimization approach, unlike the incremental stiffness approach, attempts to solve the actual nonlinear problem within a given load or time step without linearization. Accordingly, iteration

at constant load to reduce the degree of equilibrium imbalance at the end of a load or time step is not required.

Hence, it is the objective of this investigation to examine a variety of unconstrained minimization algorithms in order to determine their effectiveness for solving static and transient structural problems involving either (i) geometric nonlinearities or (ii) material nonlinearities or (iii) a combination of both geometric and material nonlinearities. Both analytic and finite difference gradients are employed with the objective of ascertaining the sensitivity of these algorithms to numerical differentiation and the computational efficacy ensuing from the use of analytic derivatives. Analytic derivatives present no insurmountable problems when only geometric nonlinearities exist. However, with material nonlinearities, the picture is radically different as the bookkeeping effort increases significantly.

The study concludes by attempting to identify the algorithm which promises to be most effective in predicting nonlinear structural response in general and suggests improvements that could be made to make it even more cost-effective when compared with other well known techniques of nonlinear structural analysis.

2. REVIEW OF THE OPEN LITERATURE

The volume and growth of available literature in the field of computer-assisted nonlinear analyses is indeed immense. Included in this mammoth collection are surveys and assessments of available computer programs for solving nonlinear structural mechanics problems [11-15]. However, "computerized nonlinear analysis is far from the black box state. The user of a general purpose nonlinear analyzer not only has to have a fairly lucid understanding of the physical sources of nonlinearity and their representation in the mathematical model, but must have some grasp of the equation formulation and equation solving process..." [16].

The scope of this investigation is to assess the performance of selected minimization techniques as applied to nonlinear structural analyses. Thus, in addition to the survey of available nonlinear minimization algorithms, it is only fitting to consider briefly the characteristics of the more conventional solution techniques for such analyses. By so doing, justification for the present investigation is provided.

2.1 Review of Conventional Solution Techniques for Nonlinear Structural Analyses

The development and evaluation of many of the conventional solution techniques documented in the open literature can be attributed to Stricklin and his associates [17-23]. Routinely, these methods

are categorized either as incremental techniques which sporadically violate equilibrium or as iterative techniques which tend to pursue the true equilibrium path. A cursory examination of the solution process of each category for nonlinear structural analysis will now be given. Interested readers should find the extensive list of references provided by Stricklin [18] extremely useful.

2.1.1 Incremental Techniques [22,24,25]

Fundamental to this approach is the incremental application of an applied load such that the character of the structure's response is essentially linear during each load or time increment for which the corresponding incremental displacements are computed. The deformed geometry of the structure is accounted for by calculating a corrective or incremental stiffness matrix. Various formulations are presented in References 26-28. The process is repeated for a specified number of load or time increments or until some previously defined maximum load or time is reached. In either case, the basic concept is to solve a sequence of linear problems with the stiffness matrices recalculated after every m load or time steps (m $\geq$ 1) in order to reflect the effects of the deformed geometry.

As a result of the ease of implementing the incremental techniques into existing linear finite element computer codes, their popularity grew. However, since equilibrium is not satisfied at any given load level without iterating at a constant load, drifting of the solution from the true equilibrium solution may be experienced if the load or

time increments are not sufficiently small and the degree of non-
linearity high. The basic concept of the incremental technique can
be seen in the incremental stiffness procedures [29,30], perturbation
methods [31,32], and initial-value formulations [33,34].

2.1.2 Iterative Techniques [22,24,25]

This approach, frequently termed self-correcting, has the salient
feature of generating solutions which satisfy equilibrium. Beginning
with an initial estimate to the displacement solution, the nonlinear
effects are calculated and an improved solution obtained by solving
a set of linearized equations. Frequently employed as an equilibrium
check is the degree of force imbalance for the calculated displace-
ment solution. This is then compared to a specified value below which
convergence or near equilibrium is defined. If the force imbalance
exceeds the prescribed value, the portion of the total loading that
is not balanced is used in the next step to determine a corresponding
increment of displacement. The procedure is repeated until the
defined near equilibrium state is achieved. The likelihood of the
solution diverging from the true equilibrium configuration is
diminished provided the time steps are small enough such that the
linearized response of the nonlinear behavior is adequate.

The method of successive approximations [18], the generalized
Newton-Raphson or tangent stiffness method [9,27,35], the modified
Newton-Raphson technique [33,36], the self-correcting initial-value
formulation [37] and the self-correcting incremental approach [38]

are representative of the iterative class of solution techniques.

Recent developments in this area have yielded a host of solution procedures which combine and/or modify the incremental and iterative methods. Such solution procedures have accelerated their convergence and have varied the equation formulation leaving few stones left unturned and much room for evaluation of their performance and accuracy.

2.2 Review of Nonlinear Minimization Algorithms

At this point, it should be realized that some of the previously described techniques linearize the structure's response within the load or time step and therefore necessitate taking small load or time steps in order to avoid diverging from the true solution. However, this is not the case with minimization algorithms. These iterative techniques solve the actual nonlinear problem within a load or time step thereby eliminating the possibility of divergence. In most cases, they should probably allow large enough load or time steps to be taken in order to compensate for any additional computational effort required by the minimization algorithm.

The study of methods which locate the minimum value of a nonlinear function, referred to as minimization algorithms, also gained considerable momentum with the advent of the digital computer. With the digital computer and a specific minimization algorithm as his tool, the analyst can test a function at a set of points which will provide information about the function and the location of its minimum. However, the minimization algorithms used to select these points can be

divided into two very general categories: nonsequential and
sequential. In the nonsequential category, these test points are
chosen randomly according to an N-dimensional probability density
function. These techniques are typically very inefficient and costly;
therefore, they are of minuscule importance [16,39] and have not been con-
sidered in this study. In the sequential category, the test points are
selected by prescribed and ordered sets of operations. Generally,
the basic procedure of a minimization algorithm is similar to the
flow diagram presented in Figure 1. Often in the literature, the
sequential category is subdivided into the direct search methods and
the gradient methods. For unconstrained problems, the gradient
methods when applicable tend to be more efficient than the direct
search methods [40]. The direct search methods require only evaluation
of the function and are classified herein as zeroth order methods.
The gradient methods encompass those which call for the evaluation
of the first derivatives in addition to evaluating the function. These
can be further classified as first order methods which do not evaluate
or approximate either the Hessian matrix or its inverse, and second
order methods which do utilize this information pertaining to the
curvatures of the function. Surveys of unconstrained minimization
techniques and comparisons of their performance are available in the
open literature [39,41-48]. Nevertheless, one must bear in mind that
the conclusions of these comparative studies were based primarily on
the number of equivalent function evaluations necessary to minimize
test functions of a purely mathematical nature. Geometric and material

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                        ┌─────────────┐
                        │    START    │
                        └─────────────┘
                               │
                               ▼
        ┌──────────────────────────────────────────────┐
        │              ESTABLISH INITIAL                │
        │                 VALUES OF                      │
        │            x_0, f_0, d_0, g_0                  │
        │  (variables, function, directions, gradient)  │
        └──────────────────────────────────────────────┘
```

START

ESTABLISH INITIAL VALUES OF $\underline{x}_0$, f_0, $\underline{d}_0$, g_0 (variables, function, directions, gradient)

ONE-DIMENSIONAL MINIMIZATION

SELECT α^* TO MINIMIZE $f(\underline{x}_i + \alpha\, \underline{d}_i)$

SET $\underline{x}_{i+1} = \underline{x}_i + \alpha^*\underline{d}_i$

CHECK CONVERGENCE $\alpha^*\underline{d}_i \leq \epsilon$

TRUE

FALSE

COMPUTE NEW DIRECTIONS $\underline{d}_{i+1}$

WRITE OUT RESULTS

STOP
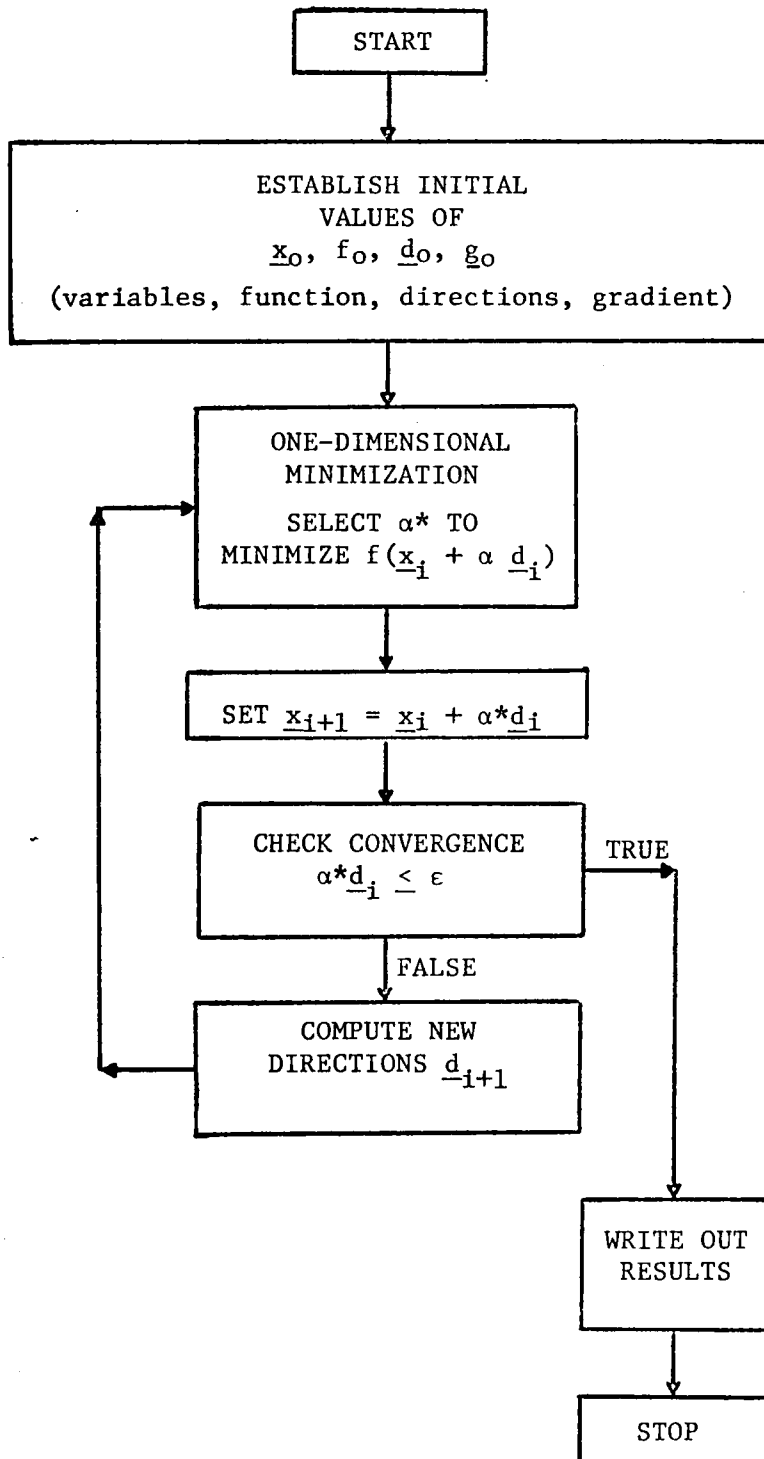
Figure 1. General Flowchart of a Typical Minimization Algorithm

nonlinearities cannot in general be described by smooth nonlinear functions of the type considered by previous investigators. An energy evaluation for an inelastic member is several times more expensive than that for a purely elastic member. Furthermore, the calculation effort involved in the function and gradient evaluations in the case of finite element models, with rather specialized connectivity properties leading to banded stiffness matrices, may bear no direct and simple relationship with those involved in the case of simple mathematical functions. The conclusion regarding the effectiveness of these algorithms for the solution of nonlinear problems of structural analyses are likely to be different. The effectiveness of these algorithms may be very much a function of the type of nonlinearity-geometric or material and also whether a static or a transient problem is being considered.

2.2.1 Zeroth Order Methods

Common to the early zeroth order methods was a heuristic or intuitive approach of selecting search directions and determining the location of the minimum function value; e.g., the alternating variable or univariate method [49], the simplex method of Himsworth, Spendley and Hext [50], the pattern search method of Hooke and Jeeves [51], and the Rosenbrock method [52]. Improvements and variations of these methods fluorished and were soon well documented in the literature. Typical of these are Nelder and Mead's simplex method [53], and the modified Rosenbrock method of Davies, Swann and Campey [54]. New methods also

emerged which were based on the properties of quadratic functions and involved successive linear minimizations along generated conjugate directions. Smith's method [55] which follows the parallel subspace approach and Powell's method of conjugate directions [56] are typical of these innovative techniques which have since served as a foundation for the more powerful techniques.

Fletcher [39] noted that on the basis of function evaluations, Powell's method is the most efficient and converges rapidly once near the minimum. Box, Davies and Swann [57] also conclude that Powell's method is the most effective zeroth order technique, particularly because of the convergence properties near the minimum. However, Nelder and Mead [53] document that their simplex method exhibits superior performance when compared with Powell's method for functions of two, three and four variables. Interestingly enough, Box [43] and Fletcher [48] both point out that this superior performance is not characteristic of Nelder and Mead's method as the number of independent variables increases.

Hence, Nelder and Mead's simplex method and Powell's modified conjugate direction method are considered the best of the zeroth order methods and were selected for examination as representative of the zeroth order methods. Also noteworthy is the significant saving in computer storage since the zeroth order methods require neither the gradient vector nor a Hessian-like $N \times N$ matrix to be stored although high computational time should be anticipated.

2.2.2 First Order Methods

First order methods, a subclass of gradient methods, incorporate gradient information in the determination of the search directions. Characteristic of many first order methods is the ease of implementation, a modest storage requirement and probably fast convergence. With these advantages, solving large problems on relatively small computers becomes quite feasible for several first order methods when used in conjunction with a linear finite element analysis [58].

The impetus behind using search directions based on the gradient vector lies in the fact that no other vector can give as great a local change in the function value [57,59]. Cauchy [60] pioneered the method of steepest descent by exploiting this property for the purpose of locating a function's minimum by searching in the direction opposite to the gradient. The demise of this technique rests in its convergence rate which has been reviewed by Akaike [61] and is often unpredictable and excruciatingly slow [44,48,57].

More powerful algorithms have been developed where the new search directions are calculated as part of the iterative scheme instead of being preassigned. Thus, any accumulated knowledge of the local behavior of the function is taken into account [62]. Capitalizing on the inherent properties of quadratic functions, the method of conjugate gradients [62,63] was developed for locating the minimum of an unconstrained function of several variables and has been used successfully on many problems. Modified versions of the conjugate gradient technique have since evolved which have modest storage

requirements [64-66].

Recently, a new algorithm based upon homogeneous rather than quadratic functions was presented by Jacobson and Oksman [67] and is reported to be quite successful for minimizing general functions [46]. Fried [68] has utilized this innovative approach in developing a new conjugate gradient method where the storage of the N x N matrix required by the Jacobson and Oksman method is avoided; however, no numerical results have been reported.

Essentially all gradient methods use the method of steepest descent to choose at least the initial search directions. For this reason and the fact that it is the classic first order method, testing of the method of steepest descent was performed, in spite of Allwright's reported superiority of the conjugate gradient method [69]. Vanderplaats' [70] version of the Fletcher and Reeves' conjugate gradient method was studied because of its modest storage requirement and because this version had previously been successfully utilized for structural analysis wherein other versions had failed. The final first order method examined was the Jacobson and Oksman method. This technique is reported to be more rigorous and superior to even second order methods [46,67]. On the other hand, only a limited amount of results have appeared for this method in the open literature.

2.2.3 Second Order Methods

Second order methods use curvature related information in addition

to the gradient vector for calculating the new search directions. This information is obtained either by evaluating and inverting the Hessian matrix directly as in the case of Newton's technique or by generating the same iteratively by capitalizing on the properties of a quadratic function and by exploiting the accumulated knowledge of the local behavior of the function.

Practically all methods in this class are related to Newton's technique. For most problems, this procedure is often very cumbersome and uneconomical, in spite of its high accuracy. Thus, numerous techniques have been developed in an attempt to circumvent these unsatisfactory features and still insure an acceptable degree of accuracy. These are referred to as quasi-Newton, pseudo-Newton or variable metric methods which use recurrence relations to update a matrix which ultimately converges to the inverse of the Hessian matrix. This variable metric serves as the metric for transforming the gradient vector into new search directions. Davidon's [71] original work was devoted to this concept which for quadratic functions generates theoretically the same identical steps as the conjugate gradient method [72]. Following its debut, there soon appeared copious variations of the method itself and of the schemes for updating the variable metric. Broyden [73,74], Huang [75], Oren [76] and Murtagh and Sargent [41] have reviewed and compared several of these updating formulae, their convergence properties and have depicted their interrelationships, particularly their relationship with Newton's method. Prominent among these second order methods are the

Davidon-Fletcher-Powell variable metric method [77,78], Davidon's variance method [79], Davidon's variable metric method with a reset option [80], Fletcher's variable metric method [81], the Goldstein-Price method [82], the Newton-Raphson method [57] and the Armstrong-Marquardt method [83,84].

Based on the number of function evaluations, Straeter and Hogge [45] report that Armstrong-Marquardt's combined steepest descent and Newton-Raphson method appears to be the superior method compared to the other methods included in their review. However, it is applicable to only a special class of functions and is not well suited for structural analysis. Some difficulties related to the Hessian matrix have been reported [45] in using the Goldstein-Price method. The popular and highly regarded Davidon-Fletcher-Powell's algorithm is noted for its ease of implementation, its fast convergence, and its requirement of significant storage [44,45,57,62,85]. It has also been noted that the Davidon-Fletcher-Powell method is often more expedient in converging than the Newton-Raphson method for large systems of equations but may fail to converge in cases where the Newton-Raphson method is successful [86]. Fletcher's new variable metric method, also derived from Davidon's work [71], is documented as exhibiting much faster convergence than the Davidon-Fletcher-Powell algorithm [46,81]. The fastest overall convergence rate has been found for Davidon's variance algorithm [45] but only a limited amount of validation is available. Unfortunately, the method requires the specification of three problem dependent parameters which dramatically

affect its performance [45,87].

Thus, the Davidon-Fletcher-Powell variable metric method, Fletcher's new variable metric method and Davidon's variance method may be regarded as being superior of the second order methods. Hence, these were selected for examination as representative of second order methods.

2.3 Summary

Based on the literature reviewed, eight techniques for unconstrained minimization of a nonlinear function of several variables were selected on the basis of their reported performance in minimizing nonlinear mathematical functions. Each technique is paraphrased in Appendix B along with citing a reference for the details of each algorithm.

3. BASIS OF THE ASSESSMENT

3.1 Solution Basis

Critical to any assessment or evaluation of the effectiveness of different techniques in solving a given problem is the establishment of a consistent and equitable comparative basis. To this end, the selected unconstrained minimization algorithms were implemented into the ACTION simulator [99] in order to achieve a uniform mathematical modelling of the problems to be solved. As shown in Appendix A, ACTION indirectly solves the equations of equilibrium of a N degree of freedom finite element model by minimizing the functional S.

$$S = \sum_{i=1}^{N} \left\{ M_i \left[\frac{3}{(\Delta t)^2} X_{ei}^2 - \left(\frac{6}{(\Delta t)^2} X_{oi} + \frac{6}{(\Delta t)} \dot{X}_{oi} \right.\right.\right.$$

$$\left.\left.\left. + 2 \ddot{X}_{oi} \right) X_{ei} \right] - F_i \Big|_{t_o + \Delta t} X_{ei} \right\} + U + C \qquad (1)$$

where M_i is the mass corresponding to the i-th degree of freedom

F_i is the exciting force corresponding to the i-th degree of freedom

U is the total strain energy

$X_{oi}, \dot{X}_{oi}, \ddot{X}_{oi}$ are the generalized displacement, velocity and acceleration, respectively, of the i-th degree of freedom at the beginning of a time step

X_{ei} is the generalized displacement of the i-th degree of freedom at the end of a time step

C is an arbitrary constant.

For linear structural analysis, this functional is a quadratic form in the unknown generalized nodal displacements of the finite element model in question. However, for nonlinear structural analysis, the same functional takes on a nonquadratic or general form.

3.2 Classification of Unconstrained Minimization Algorithms

The unconstrained minimization algorithms are broadly classified into three distinct classes stemming from the level of computational sophistication: (i) the zeroth order, requiring only function evaluations; (ii) the first order, requiring gradient as well as function evaluations; and, (iii) the second order, requiring in addition a variable metric which is used essentially as a metric for transforming the gradient direction directly into a new search direction. One remarkable facet of the variable metric is that it ultimately converges to the inverse of the Hessian matrix of Eq. (1) [90]. Under consideration are the following minimization techniques representative of each class.

1. Zeroth Order Methods

    a. Nelder-Mead's simplex method
    b. Powell's conjugate direction method

2. First Order Methods

    a. Method of steepest descent
    b. Fletcher-Reeves' conjugate gradient method
    c. Jacobson-Oksman's method

3. Second Order Methods

    a. Davidon-Fletcher-Powell's variable metric method

b. Davidon's variance method

c. Fletcher's new variable metric method

In minimizing Eq. (1), an equitable comparative basis is formed by imposing the following conditions on the minimization process:

(i.) A zero initial guess be used for the initial load or time step.

(ii.) For subsequent load or time steps, the results from the previous load or time step be used as the initial guess.

(iii.) Convergence is achieved when the nondimensionalized displacement variables change by less than 10^{-8}.

(iv.) For the second order methods, the variable metric is consistently set either to the identity matrix at the beginning of each load or time step or to the identity matrix initially and updated thereafter; that is, the variable metric at the end of a step is assumed as an initial guess for the variable metric of the next step.

Thus, the response of the finite element models with geometric and/or material nonlinearity is predicted in the same manner for all problems regardless of the minimization algorithm used.

3.3 Classification of Problems

The problems to be analyzed are arranged into five different categories stemming from the type or degree of nonlinearity and from whether the problem is static or transient. Four categories of the

static variety were chosen and include the following: (i) the
elastica problem, Figure 2, as the one involving only mild geometric
nonlinearities, $P/P_{cr} \leq 0.4$; (ii) the rod-spring problem, Figure 3,
which is geometrically moderately nonlinear; (iii) an elastic-plastic
cantilever beam subjected to a tip bending moment, Figure 4, as the
one involving only material nonlinearities (deformations and rotations
constrained to be small and geometrically linear); and, (iv) an
elastic-plastic cantilever beam subjected to a tip bending moment,
Figure 4, with rotations allowed to be moderately large. The fifth
category was of the transient variety: an impulsively loaded elastic-
plastic clamped beam, Figure 5, wherein the rotations are allowed to
be moderately large. It should be noted that the structural response
of each system as predicted by the mathematical model is in excellent
agreement with that presented by Huddleston [88] for the elastica
problem; by Haisler, Stricklin and Stebbins [19] for the static rod-
spring problem; and, by Belytschko and Schoeberle [89] for the
impulsively loaded elastic-plastic clamped beam problem. Several load
or time steps are reported for each of the above problems. This
provides an opportunity to evaluate the sensitivity of the various
algorithms to increasing nonlinearity or to changes in the partici-
pation of the geometric and material nonlinearities.

3.4 Performance Evaluation Criteria

The efficiency of these algorithms as applied to nonlinear
structural analysis is quantified by three weighting factors. These
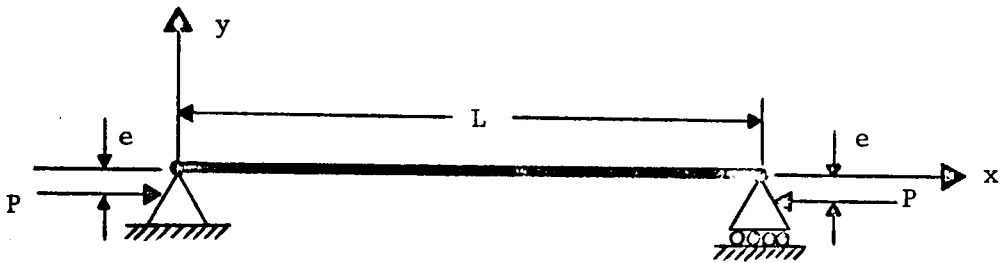
$E_{elas} = 1.958 \times 10^{11}$ Pa $\qquad$ e/L = 0.01

$A = 5.0 \times 10^{-5} m^2$ $\qquad$ L = 1.0m

$I_{yy} = 1.042 \times 10^{-10} m^4$ $\qquad$ $P_{cr} = 2.013 \times 10^2 N$

Figure 2. Elastica Problem (10 Elements, 30 Degrees of Freedom).
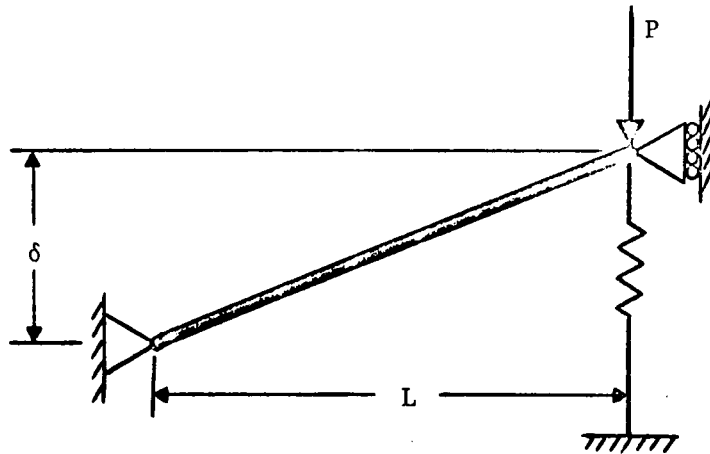
$$AE = 4.45 \times 10^7 N \qquad\qquad \Delta P = 4.45N$$

$$L = 2.54m \qquad\qquad\qquad k_s = 1050N/m$$

$$\delta = 2.54cm$$

Figure 3. Rod-Spring Problem (5 Elements, 12 Degrees of Freedom.)
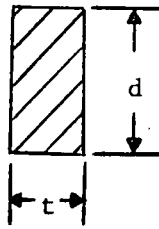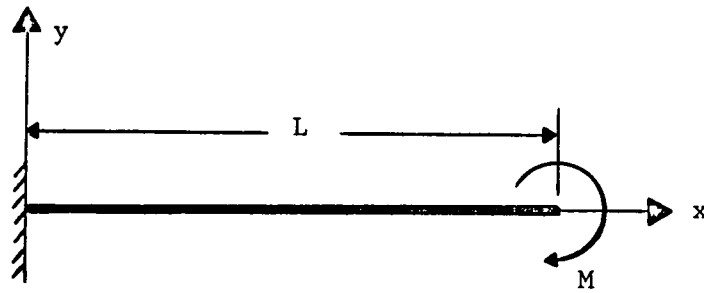
$E_{elas} = 1.958 \times 10^{11}$ Pa

$E_{plas} = 3.751 \times 10^{8}$ Pa

$\sigma_{yp} = 5.585 \times 10^{8}$ Pa

$d = 1.0$ cm

$t = 0.5$ cm

$A = 5.0 \times 10^{-5} m^{2}$

$L = 1.0$ m

$I_{yy} = 4.167 \times 10^{-10} m^{4}$

$M_{yp} = 46.542$ J

Figure 4. Elastic-Plastic Cantilever Beam
(4 Elements, 12 Degrees of Freedom,
Solid Rectangular Cross Section).
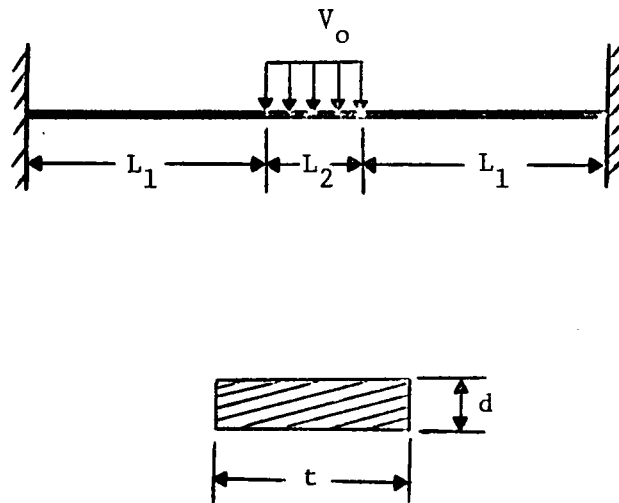
L_1 = 127mm

L_2 = 51mm

V_o = 51.18m/sec.

ρ = 7870kg/m^3

E_{elas} = 1.958x10^{11}Pa

E_{plas} = 3.751x10^{8}Pa

σ_{yp} = 5.585x10^{8}Pa

d = 3.18mm

t = 25.40mm

Figure 5.   Impulsively Loaded Elastic-Plastic Clamped Beam (10 Elements Over Half the Span, 28 Degrees of Freedom, Solid Rectangular Cross Section).

factors have been normalized to their respective minimum value per

load or time step, such that the most efficient algorithm will have

weighting factors of 1.00. Two of the factors are the number of

minimizations and the amount of CPU time required per load or time

step. Unlike the previous two factors, the third factor is dependent

on the order of the minimization algorithm in the sense that all of

these algorithms do not require evaluation of the gradient vector.

Therefore, in order to sanction an inter-class as well as an intra-

class assessment of the zeroth, first and second order algorithms,

a factor which is a composite of the number of function and gradient

evaluations was defined and termed the number of equivalent member

energy evaluations. The determination of this factor depends on how

the gradients are calculated. For analytic gradients, approximately

one equivalent member energy evaluation for each degree of freedom of

the structure being analyzed is required to obtain the gradient

vector. However using the central difference operator, each component

of the gradient vector corresponding to any one nodal degree of freedom

requires at least two equivalent member energy evaluations, four if

that node is common to two elements, six if it is common to three

elements, etc. Hence, a significant reduction in the number of

equivalent member energy evaluations and in CPU time should be

realized if analytic gradients are used as required by the first and

second order algorithms. Appendix C outlines the development of the

analytic gradient for frame elements with geometric and/or material

nonlinearities.

3.5 Summary

The selected unconstrained minimization algorithms were adapted to the ACTION simulator in order to investigate their performance when applied to nonlinear structural analyses using finite element modelling. Also, an analytic gradient feature was added to ACTION which previously calculated the gradient by using finite difference operators. Hence, both analytic and finite difference gradients are used with a view to determining the sensitivity of these algorithms to inaccuracies in the gradient evaluations and to determine the computational efficiency ensuing from the use of analytic gradients.

All numerical results were generated by the ACTION simulator using the IBM System/370 Model 158 computer and accompanying peripheral equipment wherein double precision arithmetic (sixteen significant digits) is used throughout. It should be realized that slight variations in CPU time are possible due to variations in the system's multi-processor unit. Therefore, the weighting factors related to the required CPU time and the number of equivalent member energy evaluations need to be considered simultaneously in order to avoid any misinterpretation of the results reported herein. Thus, consistent and equitable guidelines for this assessment have been established.

4. RESULTS AND CONCLUSIONS

4.1 Discussion of Results Using Finite Difference Gradients

For most minimization algorithms using finite difference approximations to the gradients, the computational effort required to evaluate the gradient using a central difference operator may be nearly twice that required for either a forward or backward difference operator. This computational advantage is partially offset by the fact that the accuracy of the derivatives obtained by utilizing the forward or backward difference operator is likely to be poor. Limited studies have indicated that for first order methods considerable savings in computational time may be realized for some problems by using forward or backward difference derivatives. It is tacitly assumed however that for the calculation of such derivatives, stepsizes must be much smaller (approximately 1/100th to 1/1000th; with the minimum being the precision of the computer) than the stepsizes used for central difference derivatives. The same computational advantage may not be realized with second order methods utilizing a variable metric which is updated recursively using current function and gradient information. In this case, the inaccuracies in the variable metric resulting from forward or backward difference derivatives can retard the convergence rate substantially, thus offsetting the savings accrued from the relatively cheaper gradient evaluation. For second order methods, the only time forward or backward difference derivatives appear to be competitive with central difference derivatives is when the initial

variable metric is set equal to the identity matrix at the beginning of each load or time step of a nonlinear analysis. That is to say, the variable metric at the end of a load or time step is not carried forward as the initial variable metric of the next step. It is therefore concluded that the performance of most minimization algorithms employing forward or backward difference derivatives is unpredictable and quite sensitive to the type and degree of nonlinearity in question, even more so than with central difference derivatives. Hence, their use should be avoided whenever possible.

For the results reported in Tables 2 through 6, all gradients were evaluated using a central difference operator. Furthermore, one of the results not reported in the Table 2 is that of a fifteen (15) degree of freedom model of the elastica problem for which the zeroth order conjugate direction method was found to be more efficient than even a second order method like the Davidon-Fletcher-Powell method. For large degree-of-freedom systems, the conjugate direction method is well known not to be nearly as efficient because of the generation of very nearly dependent directions. This is borne out by the results of the thirty (30) degrees of freedom model of the elastica problem reported in Table 2.

The effects of geometric nonlinearities on the computational effort required by the various algorithms can be observed in Table 2 for a mildly nonlinear problem and in Table 3 for a moderately nonlinear problem. While none of the first order methods considered were competitive, Powell's conjugate direction method presents stiff

Table 2. Performance Data for the Elastica Problem
Using Central Difference Gradients.

MINIMIZATION ALGORITHM		APPLIED AXIAL LOAD, P/P_{cr}			
		0.1	0.2	0.3	0.4
Nelder-Mead's	(m)	91.53*	–	–	–
Simplex	(e)	4.42	–	–	–
Method	(t)	3.99	–	–	–
Powell's Conjugate	(m)	1.00	7.91	7.00	6.14
Direction	(e)	2.38	36.78	32.12	28.13
Method	(t)	2.05	27.80	25.61	21.82
Fletcher-Reeves' Method	(m)	3.14	24.45	45.83*	–
with restarts after the	(e)	2.30	31.13	55.51	–
first N+2 iterations only.	(t)	1.96	23.40	42.06	–
Method of	(m)	2.54	17.91	17.58**	–
Steepest	(e)	1.82	22.78	20.90	–
Descent	(t)	1.47	17.15	16.72	–
Jacobson-Oksman's	(m)	1.76	33.09	28.58*	–
Method	(e)	1.71	69.17	60.21	–
	(t)	1.45	55.03	50.39	–
Davidon's Variance	(m)	3.39*	–	–	–
Method with	(e)	2.74	–	–	–
$\underline{H}_o=\underline{I}$	(t)	1.51	–	–	–
Davidon's Variance	(m)	3.22	17.27	26.00*	–
Method with $\underline{H}_o=\kappa\underline{I}$	(e)	1.51	16.00	23.41	–
where $\kappa=0.1$	(t)	1.46	13.42	20.61	–
Fletcher's Method	(m)	3.78	40.73	31.08	28.14
with $\underline{H}_o=\underline{I}$ always.	(e)	1.77	37.50	28.12	25.56
	(t)	1.59	30.64	23.45	20.62
Fletcher's Method	(m)	3.78	1.00	2.00	2.00
with $\underline{H}_o=\underline{I}$ only	(e)	1.79	1.00	1.87	1.85
initially.	(t)	1.79	1.00	1.72	1.72
Davidon-Fletcher-	(m)	1.53	9.18	13.58	11.21
Powell's Method with	(e)	1.00	11.82	17.04	14.21
$\underline{H}_o=\underline{I}$ always.	(t)	1.04	11.44	15.49	12.84
Davidon-Fletcher-	(m)	1.53	1.64	1.00	1.00
Powell's Method with	(e)	1.00	1.91	1.00	1.00
$\underline{H}_o=\underline{I}$ only initially.	(t)	1.00	1.79	1.00	1.00

*Failed to converge

**Converged but analysis terminated

(m)...Weighting factor for the number of minimizations.
(e)...Weighting factor for the number of equivalent member energy
     evaluations.
(t)...Weighting factor for the required CPU time.

Table 3. Performance Data for the
Rod-Spring Problem Using
Central Difference Gradients.

MINIMIZATION ALGORITHM		RESULTS FROM THIRTY (30) LOAD STEPS
Powell's	(m)	3.08
Conjugate	(e)	7.02
Method	(t)	5.40
Fletcher's Method with	(m)	1.57
$H_o = I$ only initially	(e)	1.47
	(t)	1.34
Davidon-Fletcher-Powell's	(m)	1.00
Method with $H_o = I$ only	(e)	1.00
initially	(t)	1.00

(m)...Weighting factor for the number of minimizations.
(e)...Weighting factor for the number of equivalent member energy
    evaluations
(t)...Weighting factor for the required CPU time.

competition to Fletcher's method which sets the initial variable metric to the identity matrix at the beginning of each load step. For the degree of geometric nonlinearity considered, the Davidon-Fletcher-Powell method using an updated variable metric is more efficient. However, as the degree of nonlinearity continues to increase, Fletcher's method using an updated variable metric becomes the superior technique. Also, the computational advantage of second order methods which update the variable metric recursively over those which do not can be readily seen in Table 2.

The effects of material nonlinearities arising from loading and unloading while in the inelastic range can be seen in Table 4. For this study, a linear elastic response is considered for the first two loading steps, followed by two loading steps in the inelastic range and a final unloading step back into the elastic range. For the linear elastic portion where Eq. (1) has a quadratic form, all methods performed at least marginally well with the exception of Nelder-Mead's method and the method of steepest descent which performed poorly. An unexpected result came from the fact that the Jacobson-Oksman algorithm had to be repeatedly restarted to ensure linear independence of the search directions. This is reported to have never been necessary Jacobson and Oksman [67] for their test functions.

Although initially superior for the linear elastic steps, the Davidon-Fletcher-Powell method is less competitive than Powell's conjugate direction method (a zeroth order method) for inelastic loading. Fletcher's method is very sluggish in finding a solution

Table 4. Performance Data for an Elastic-Plastic Cantilever Beam Subjected to a Tip Bending Moment with Small and Geometrically Linear Deformations and Rotations Using Central Difference Gradients.

MINIMIZATION ALGORITHM		APPLIED TIP BENDING MOMENT, M/M_{yp}				
		0.215	1.074	1.289	1.397	1.289
Nelder-Mead's	(m)	360.82*	–	–	–	–
Simplex	(e)	18.73	–	–	–	–
Method	(t)	13.63	–	–	–	–
Powell's Conjugate	(m)	1.00	3.00	1.00	1.00	2.44
Direction	(e)	1.83	10.59	2.16	1.74	5.75
Method	(t)	1.44	4.25	1.86	1.70	4.97
Fletcher-Reeves' method	(m)	2.18	6.25	10.31*	–	–
with restart after the	(e)	1.22	7.06	9.54	–	–
first N+2 iterations only	(t)	1.00	2.99	10.84	–	–
Method of	(m)	272.73*	–	–	–	–
Steepest Descent	(e)	146.95	–	–.	–	–
	(t)	89.89	–	–	–	–
Davidon's Variance	(m)	8.18	26.25	14.06*	–	–
Method with	(e)	3.51	22.57	9.72	–	–
$H_o = \kappa I$ where κ=0.1	(t)	2.40	8.53	8.86	–	–
Fletcher's Method	(m)	9.45	1.75	1.17	1.44	2.67
with H_o=I only	(e)	4.28	2.13	1.00	1.00	3.09
initially	(t)	3.20	1.34	1.00	1.00	2.82
Davidon-Fletcher-Powell's	(m)	1.55	1.00	2.29	3.52	1.00
Method with H_o=I only	(e)	1.00	1.00	2.09	2.67	1.00
initially	(t)	1.02	1.00	2.49	2.65	1.00

*Failed to Converge

(m)...Weighting factor for the number of minimizations.
(e)...Weighting factor for the number of equivalent member energy evaluations.
(t)...Weighting factor for the required CPU time.

during elastic loading. This is as expected in that methods which utilize the property of quadratic termination will be more efficient for problems involving quadratic functionals than Fletcher's method which discards this property. Fletcher's method is superior during inelastic loading, while the superiority of the Davidon-Fletcher-Powell method is regained when unloading occurs and overall it is again the more efficient method.

Table 5 summarizes the computational effort expended in solving a problem with a high degree of geometric and material nonlinearities. Of the methods tested, only Fletcher's method was successful in solving this problem within a reasonable amount of computer time for the specified load steps. For this case, Davidon-Fletcher-Powell's method gets hung-up during the first load step in the inelastic range. With geometric nonlinearities, Eq. (1) becomes nonquadratic even for the elastic case. Hence, the performance of Fletcher's method is as anticipated; that is to say, better than that of the Davidon-Fletcher-Powell method.

Table 6 represents the results from a transient problem wherein, to a moderate degree, both geometric and material nonlinearities were included. Again overall superiority was demonstrated by Fletcher's method using an updated variable metric.

4.2 Discussion of Results Using Analytic Gradients

It can be seen that these minimization algorithms are more sensitive to geometric nonlinearities than to material nonlinearities.

Table 5. Performance Data for an Elastic-Plastic Cantilever Beam Subjected to a Tip Bending Moment with Moderately Large Rotations Using Central Difference Gradients.

MINIMIZATION ALGORITHM		APPLIED TIP BENDING MOMENT, M/M_{yp}				
		0.215	1.074	1.289	1.397	1.289
Powell's Conjugate	(m)	1.00	2.48**	–	–	–
Direction	(e)	1.18	5.62	–	–	–
Method	(t)	1.10	5.14	–	–	–
Fletcher-Reeves' method	(m)	4.91	14.33**	–	–	–
with restart after the	(e)	3.03	16.21	–	–	–
first N+2 iterations only	(t)	2.75	14.89	–	–	–
Davidon's Variance	(m)	17.24*	–	–	–	–
Method with	(e)	7.21	–	–	–	–
$H_o=\kappa I$ where $\kappa=0.1$	(t)	6.78	–	–	–	–
Fletcher's Method	(m)	2.28	1.48	1.00	1.00	1.00
with $H_o=I$ only	(e)	1.00	1.35	1.00	1.00	1.00
initially	(t)	1.00	1.30	1.00	1.00	1.00
Davidon-Fletcher-Powell's	(m)	10.47	1.00	2.34*		
Method with $H_o=I$ only	(e)	6.05	1.00	2.83		
initially	(t)	6.02	1.00	3.12		

*Failed to converge

**Converged but analysis terminated

(m)...Weighting factor for the number of minimizations.
(e)...Weighting factor for the number of equivalent member energy evaluations.
(t)...Weighting factor for the required CPU time.

Table 6. Performance Data for an Impulsively
Loaded Elastic-Plastic Clamped
Beam with Moderately Large
Rotations Using Central Difference
Gradients.

MINIMIZATION ALGORITHM		TIME (IN GROUPS OF TEN TIME STEPS; $t_o=0.0$, $\Delta t=10^{-6}$ SECONDS)			
		I	II	III	IV
Nelder-Mead's	(m)	135.41*	–	–	–
Simplex	(e)	6.44	–	–	–
Method	(t)	2.44	–	–	–
Powell's Conjugate	(m)	1.00	1.26†	–	–
Direction	(e)	2.55	5.92	–	–
Method	(t)	1.77	4.05	–	–
Fletcher-Reeves' Method	(m)	5.41	10.37†	–	–
with restart after the	(e)	2.93	8.15	–	–
first N+2 iterations only.	(t)	2.13	7.10	–	–
Method of	(m)	21.89†	–	–	–
Steepest	(e)	11.75	–	–	–
Descent	(t)	7.12	–	–	–
Davidon's Variance	(m)	15.07**	–	–	–
Method with $H_{-o}=\kappa I$	(e)	6.63	–	–	–
where $\kappa=0.1$	(t)	4.15	–	–	–
Fletcher's Method with	(m)	2.52	1.00	1.00	1.00
$H_{-o}=I$ only initially	(e)	1.53	1.00	1.00	1.00
	(t)	1.07	1.00	1.00	1.00
Davidon-Fletcher-	(m)	2.00	2.39	3.46	2.02
Powell's Method with	(e)	1.00	2.08	3.26	1.96
$\underline{H}_o=\underline{I}$ only initially	(t)	1.00	1.91	2.65	1.69

*Failed to converge at $t=6.0 \times 10^{-5}$ seconds

**Failed to converge at $t=9.0 \times 10^{-5}$ seconds

† Converged but analysis terminated

(m)...Weighting factor for the number of minimizations.
(e)...Weighting factor for the number of equivalent member energy
    evaluations.
(t)...Weighting factor for the required CPU time.

Furthermore, the above results together with the experiments with
finite difference derivatives clearly indicate that all first and
second order algorithms are critically influenced by the accuracy of
the gradient. This leads very naturally to the consideration of
analytically derived gradient vectors and of their effectiveness.
The performance of the first and second order methods using analytic
gradients is reported in Tables 7 through 9.

The effects of geometric nonlinearities on the computational
effort required can be observed in Table 7 for a mildly nonlinear problem
and in Table 8 for a highly nonlinear problem. These results again
indicate the superior performance of the second order methods. Also,
as the degree of geometric nonlinearity increases or in other words,
Eq. (1) becomes more nonquadratic, the superiority of Fletcher's method
over the Davidon-Fletcher-Powell method becomes more and more evident.
It should also be noted that Fletcher-Reeves' method using analytic
gradients is able to converge for all load steps considered whereas
using central difference gradients, it was not.

The effects of material nonlinearities are reported in Table 9.
For this study, two elastic and two inelastic loading steps are made.
For the linear elastic portion, the results correlate well with those
reported in Table 4. However, for inelastic loading, Davidon-
Fletcher-Powell's method maintained its superiority over Fletcher's
method. This is quite interesting in that a definite change in per-
formance is observed from that reported in Table 4. In switching
from difference derived gradients to analytic gradients, the performance

Table 7. Performance Data for the Elastica
Problem Using Analytic Gradients

Minimization Algorithm		Applied Axial Load, P/P_{cr}			
		0.1	0.2	0.3	0.4
Fletcher-Reeves'	(m)	2.27	16.82	15.06	22.54
Method with Restarts	(e)	2.80	34.69	20.94	32.31
After the First N+2	(t)	1.99	17.96	12.13	16.23
Iterations Only					
Fletcher's Method	(m)	2.97	1.00	1.41	2.15
with $H_o = I$ Only	(e)	1.35	1.00	1.00	1.63
Initially	(t)	1.36	1.00	1.00	1.30
Davidon-Fletcher-	(m)	1.00	1.27	1.00	1.00
Powell's Method with	(e)	1.00	1.81	1.22	1.00
$H_o = I$ Only Initially	(t)	1.00	1.67	1.16	1.00

(m)... Weighting factor for the number of minimizations.
(e)... Weighting factor for the number of equivalent member energy
    evaluations.
(t)... Weighting factor for the required CPU time.

Table 8. Performance Data for an Elastic
Cantilever Beam Subjected to a
Tip Bending Moment with
Moderately Large Rotations
Using Analytic Gradients

Minimization Algorithm		Applied Tip Bending Moment, M/M_{yp}	
		0.215	1.074
Fletcher's Method	(m)	1.00	1.23
with $H_o = I$ Only	(e)	1.00	1.00
Initially	(t)	1.00	1.00
Davidon-Fletcher-	(m)	3.66	1.00
Powell's Method	(e)	7.33	1.24
with $H_o = I$ Only	(t)	6.64	1.27
Initially			

(m)... Weighting factor for the number of minimizations.
(e)... Weighting factor for the number of equivalent member energy
      evaluations.
(t)... Weighting factor for the required CPU time.

Table 9. Performance Data for an Elastic-Plastic
Cantilever Beam Subjected to a Tip
Bending Moment with Small and Geo-
metrically Linear Deformations and
Rotations Using Analytic Gradients.

Minimization Algorithm		Applied Tip Bending Moment, M/M_{yp}			
		0.215	1.074	1.289	1.397
Fletcher-Reeves'	(m)	2.83	19.00	150.20*	--
Method with Restart	(e)	2.12	21.14	139.81	--
After the First N+2	(t)	1.42	3.19	104.15	--
Iterations Only					
Fletcher's Method	(m)	8.67	3.50	1.20	1.00
with $\underline{H}_o = \underline{I}$ Only	(e)	3.43	2.29	3.79	4.75
Initially	(t)	2.46	1.25	2.38	2.12
Davidon-Fletcher-	(m)	1.00	1.00	1.00	2.00
Powell's Method with	(e)	1.00	1.00	1.00	1.00
$\underline{H}_o = \underline{I}$ Only Initially	(t)	1.00	1.00	1.00	1.00

*Failed to converge.

(m)... Weighting factor for the number of minimizations.
(e)... Weighting factor for the number of equivalent member energy
    evaluations.
(t)... Weighting factor for the required CPU time.

of all first and second order methods is indeed markedly improved. However, for problems with strictly material nonlinearities such improvement in the case of the Davidon-Fletcher-Powell method in particular appears to be all the more dramatic.

4.3 Analytic Gradients Versus Central Difference Gradients

The sensitivity of the first and second order algorithms to inaccuracies in the gradient calculation and the computational savings ensuing from the use of analytic gradients is reported in Tables 10 through 12. These results clearly indicate that a significant reduction of the computational effort can be realized by using an analytically derived gradient vector. This reduction is the result of not only a cheaper gradient calculation but in most cases, a faster convergence to the solution because of the higher accuracy of all computed quantities. Perhaps the most dramatic reduction occurs in Table 12 for the inelastic loading steps. It is here that the second order methods are found to be much more sensitive to inaccurate gradients than for the case with geometric nonlinearities alone.

4.4 Conclusions and Recommendations

The performance of the selected unconstrained minimization algorithms has been summarized with regards to their effectiveness in predicting nonlinear structural response. Based on the data reported, Powell's conjugate direction method is the only zeroth order method which demonstrated good performance particularly when only

Table 10. Ratio of the Computational Effort
with Analytic Gradients to That
of Central Difference Gradients
for the Elastica Problem.

Minimization Algorithm		Applied Axial Load, P/P_{cr}			
		0.1	0.2	0.3	0.4
Fletcher-Reeves'	(m)	0.919	0.688	0.952[*]	1.089[*]
Method with Restarts	(e)	0.518	0.359	0.452	0.495
After the First N+2	(t)	0.467	0.322	0.404	0.456
Iterations Only					
Fletcher's Method	(m)	1.000	1.000	1.000	1.000
with $H_o = I$ Only	(e)	0.320	0.323	0.323	0.323
Initially	(t)	0.347	0.419	0.417	0.384
Davidon-Fletcher-	(m)	0.833	0.778	1.417	0.929
Powell's Method with	(e)	0.424	0.306	0.736	0.367
$H_o = I$ Only Initially	(t)	0.460	0.390	0.834	0.512

[*]Convergence was not achieved for the third load step using central
difference gradients; therefore, the central difference results of
the second load step were used in calculating this ratio.

(m)... Ratio of the number of minimizations.
(e)... Ratio of the number of equivalent member energy evaluations.
(t)... Ratio of the required CPU time.

Table 11. Ratio of the Computational Effort
with Analytic Gradients to That
of Central Difference Gradients
for an Elastic Cantilever Beam
Subjected to a Tip Bending Moment
with Moderately Large Rotations.

Minimization Algorithm		Applied Tip Bending Moment, M/M_{yp}	
		0.215	1.074
Fletcher's Method	(m)	0.992	0.939
with $H_o = I$ Only	(e)	0.345	0.323
Initially	(t)	0.355	0.331
Davidon-Fletcher-	(m)	0.789	1.136
Powell's Method	(e)	0.419	0.539
with $H_o = I$ Only	(t)	0.391	0.546
Initially			

(m)... Ratio of the number of minimizations.
(e)... Ratio of the number of equivalent member energy evaluations.
(t)... Ratio of the required CPU time.

Table 12. Ratio of the Computational Effort with
Analytic Gradients to That of Central
Difference Gradients for an Elastic-
Plastic Cantilever Beam Subjected to
a Tip Bending Moment with Small and
Geometrically Linear Deformations
and Rotations.

Minimization Algorithm		Applied Tip Bending Moment, M/M_{yp}			
		0.215	1.074	1.289	1.397
Fletcher-Reeves'	(m)	0.923	1.074	--*	--
Method with Restart	(e)	0.541	0.624	--	--
After the First N+2	(t)	0.618	0.625	--	--
Iterations Only					
Fletcher's Method	(m)	1.000	0.778	0.345	0.129
with $H_o = I$	(e)	0.412	0.240	0.276	0.091
Initially	(t)	0.478	0.316	0.081	0.052
Davidon-Fletcher-	(m)	0.550	0.286	0.105	0.200
Powell's Method with	(e)	0.358	0.148	0.076	0.102
$H_o = I$ Only	(t)	0.529	0.438	0.077	0.094
Initially					

*Failed to converge using both analytic and central difference
gradients.

(m)... Ratio of the number of minimizations.
(e)... Ratio of the number of equivalent member energy evaluations.
(t)... Ratio of the required CPU time.

material nonlinearities were considered. None of the first order

methods considered were competitive and in general, their use is not

recommended for nonlinear structural analysis. Despite inaccuracies

in the variable metric due to central difference derivatives, the

second order methods which utilize a variable metric are the more

efficient algorithms primarily because they exploit the curvature

related information of the function. Davidon's variance algorithm

is not recommended for general structural analysis because of its

critical dependence on three user supplied parameters. When mild

geometric or material nonlinearities are considered separately, the

Davidon-Fletcher-Powell method is found to be more cost-effective on

an overall basis over the range of load or time steps considered

herein. However, it is found that overall Fletcher's method surpasses

the Davidon-Fletcher-Powell method when geometric and material non-

linearities are combined for both static and transient problems. The

results indicate that with time and an increasing degree of geometric

nonlinearity, Fletcher's method becomes increasingly cost-effective.

The sensitivity of the first and second order algorithms to

numerical differentiation and the computational efficacy ensuing from

the use of analytic derivatives was also determined. The use of the

central difference operator for the gradient calculation will result

in more accurate derivatives than either a forward or backward

difference operator which offers a cheaper gradient evaluation. The

use of analytic gradients results in a substantial savings in

computational effort because of cheaper and more accurate derivatives.

Therefore, the following recommendations can be made. For general nonlinear structural analysis, Fletcher's new variable metric method using an updated variable metric and, if possible, analytic gradients is highly recommended. Since Fletcher's method is initially slow in converging to a solution, it is recommended that further studies centered around a more appropriate choice for the initial variable metric be conducted. If the degree of the nonlinearity is mild and only one type of nonlinearity is considered, the Davidon-Fletcher-Powell variable metric method using an updated variable metric and, if possible, analytic gradients is preferred. If an analytic gradient is unavailable, then a central difference gradient should be used. The use of a either forward or backward difference gradient should be avoided.

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APPENDICES

APPENDIX A

DESCRIPTION OF ACTION

ACTION is a computer simulator for performing transient nonlinear analysis of a geometrically complex structure utilizing the displacement formulation of the finite element technique. ACTION's approach to the prediction of nonlinear structural response is by the minimization of a scalar function of the structural characteristics with the equilibrium configuration of the model being established at the stationary values of this scalar function. For transient analyses, this formulation couples the Newmark-Beta method [8] of integrating the equations of motion with a functional minimization procedure to find a stable equilibrium configuration for discrete points within the specified temporal domain. The nonlinearities considered stem from two sources. One being the geometric nonlinearities arising from large rotations with small strains and the other arising from the inelastic response of the model characterized by a linear elastic material model with strain hardening in the inelastic range. Successful utilization of this approach for both static and dynamic nonlinear structural analysis has been documented by several investigators [95-99].

Finite element analysis using the functional minimization approach consists of the following steps as described by Kamat, Killian, Melosh and Swift [99]:

(1.) Assume a suitable element displacement field as a function

of the local spatial coordinates with the generalized

joint displacements as unknown coefficients. The displace-

ment field chosen is kinematically admissible and provides

a Ritz formulation of the discretized system.

(2.)   Relate the element generalized displacements to the global

generalized displacements of the system accounting for

prescribed boundary conditions. Using the convected

coordinate formulation [96, 99-104], the total displacement

vector is expressed as the sum of a rigid body motion and

a strain producing portion. Thus, the effects of any

geometric nonlinearity are handled entirely by the trans-

formation of the generalized displacements and forces from

the convected coordinate system to the global coordinate

system.

(3.)   Develop the expression for strains in each element as

functions of the global generalized displacements.

(4.)   Determine the corresponding strain energy density of each

of the elements using their respective material models.

(5.)   Integrate the strain energy densities over the volume of

their respective element using the Gauss-Legendre

quadrature method. This yields the element strain energy

as a function of the global generalized displacements.

(6.)   For transient analysis, the displacement-time relation

for each variable is assumed to be a linear variation of

acceleration over the time step [8]. That is,

$$X_{ei} = a_i + b_i(\Delta t) + \frac{1}{2} c_i(\Delta t)^2 + \frac{1}{6} \beta_i(\Delta t)^3$$

where X_{ei} is the i-th generalized displacement at the end of the time step and a_i, b_i, c_i and β_i are constants which are determined in terms of the generalized displacement X_{oi}, velocity $\dot{X}_{oi}$, and acceleration $\ddot{X}_{oi}$ at the beginning of the time step and the generalized displacement X_{ei} at the end of the time step. Thus,

$$a_i = X_{oi} \qquad\qquad b_i = \dot{X}_{oi} \qquad\qquad c_i = \ddot{X}_{oi}$$

$$\beta_i = \frac{6}{(\Delta t)^3} \left[(X_{ei} - X_{oi}) - \dot{X}_{oi}(\Delta t) - \frac{1}{2} \ddot{X}_{oi}(\Delta t)^2 \right]$$

Knowing the values of the generalized displacements, velocities and accelerations at the beginning of a time step, the velocities and accelerations at the end of a time step can be expressed purely in terms of the unknown generalized displacements at the end of a time step. Thus,

$$\dot{X}_{ei} = \dot{X}_{oi} + \ddot{X}_{oi}(\Delta t) + \frac{3}{(\Delta t)} \left[(X_{ei} - X_{oi}) \right.$$
$$\left. - \dot{X}_{oi}(\Delta t) - \frac{1}{2} \ddot{X}_{oi}(\Delta t)^2 \right]$$

$$\ddot{X}_{ei} = \ddot{X}_{oi} + \frac{6}{(\Delta t)^2} \left[(X_{ei} - X_{oi}) - \dot{X}_{oi}(\Delta t) \right.$$
$$\left. - \frac{1}{2} \ddot{X}_{oi}(\Delta t)^2 \right]$$

(7.) Calculate the potential of the externally applied generalized forces.

(8.) Construct a potential function for the entire system as a
function of the unknown generalized displacements. This
potential function will be the total potential energy
of the system for static analyses and Lagrangian of the
system for transient analyses with an assumed relationship
between displacements and time. The first variation of the
potential function used by ACTION gives the required
equations of equilibrium. Knowing the generalized dis-
placements, velocities and accelerations at the beginning
of a time step, the equations of equilibrium in terms of
the unknown generalized displacements at the end of a
time step take the form

$$M_i \left[\frac{6}{(\Delta t)^2} (X_{ei} - X_{oi}) - \frac{6}{(\Delta t)} \dot{X}_{oi} - 2 \ddot{X}_{oi} \right]$$

$$- F_i \Big|_{t_o + \Delta t} + \frac{\partial U}{\partial X_{ei}} = 0 \quad i = 1, 2, \ldots, N \qquad (A.1)$$

where M_i, F_i and U are the mass, exciting force and strain
energy for the i-th degree of freedom of a system of N
degrees of freedom.

(10.) This function can be developed by integrating the equations
of equilibrium considering the generalized displacements
at the end of a time step, X_{ei}, as the independent variables.
Therefore,

$$S = \sum_{i=1}^{N} \left\{ M_i \left[\frac{3}{(\Delta t)^2} X_{ei}^2 - \left(\frac{6}{(\Delta t)^2} X_{oi} + \frac{6}{(\Delta t)} \dot{X}_{oi} \right） \right. \right.$$

$$\left. + 2 \ \ddot{X}_{oi} \right) X_{ei} \Big] - F_i \Big|_{t_o + \Delta t} X_{ei} \right\} + U + C \qquad\qquad (A.2)$$

where C is a constant of integration. Based on the fact that the space spanned by the functional S is convex due to the inertial masses always being positive and the strain energy for most structural materials being a positive semi-definite function, it can be shown that Eq. (A.1) are the necessary conditions for S to take on a minimum value.

(11.) Finally, with the aid of well established minimization algorithms, the generalized displacements which correspond to a stable equilibrium configuration with minimum equilibrium imbalance are obtained through the minimization of the functional S.

The brief outline of the general flow of the ACTION simulator alluded to above is presented for completeness of presentation with the details of the theoretical formulation being available in Reference 99.

APPENDIX B

MINIMIZATION TECHNIQUES INVESTIGATED

B.1 Introduction

The majority of the minimization techniques considered in this study hypothesize that the function to be minimized has a quadratic form. The rationale of this hypothesis is revealed by examining the Taylor series expansion of a general function of N variables $f(\underline{x})$ about its minimum point $\underline{x}_m$. That is,

$$f(\underline{x}) \sim f(\underline{x}_m) + \sum_{k=1}^{N} \left[\frac{\partial f}{\partial x_k} \right]_{\underline{x}_m} (x_k - x_{mk})$$

$$+ \frac{1}{2!} \sum_{i=1}^{N} \sum_{j=1}^{N} \left[\frac{\partial^2 f}{\partial x_i \partial x_j} \right]_{\underline{x}_m} (x_i - x_{mi})(x_j - x_{mj})$$

$$+ \text{higher order terms} \qquad\qquad (B.1)$$

or in vector form

$$f(\underline{x}) \sim a + \underline{b}^T(\underline{x} - \underline{x}_m) + \frac{1}{2!} (\underline{x} - \underline{x}_m) \underline{A}(\underline{x} - \underline{x}_m)$$

$$+ \text{higher order terms} \qquad\qquad (B.2)$$

Since at the minimum point $\underline{x}_m$ the gradient vanishes and the term $|\underline{x} - \underline{x}_m|$ approaches zero, the higher order terms become relatively insignificant thereby causing the Taylor series expansion of $f(\underline{x})$ to be dominated by the constant, linear and quadratic terms in the

proximity of the minimum. This suggests that in the neighborhood of the minimum, many general functions can be approximately represented by a quadratic. The function to be minimized in this study is Eq. (1) which is discussed in Appendix A.

A prevalent feature of the techniques considered is the replacement of an N-dimensional minimization problem with a sequence of one-dimensional or linear minimizations along the line

$$\underline{x}_{k+1} = \underline{x}_k + \alpha \; \underline{d}_k \qquad\qquad (B.3)$$

such that $f(\underline{x}_{k+1})$ becomes a function of α alone when the variables $\underline{x}_k$ and the search direction $\underline{d}_k$ are both known.

The method utilized for the linear minimization depends on the computational sophistication of the particular algorithm invoked. If gradient information is available, Davidon's cubic interpolation method [71,91,92] is employed; if not, Powell's quadratic interpolation method [56,91,92] is engaged. Powell's method finds the minimum of a quadratic which is described by the values of the function at three points on the line specified by Eq. (B.3). On the other hand, Davidon's method minimizes a cubic which is defined by the values of the function and its directional derivative at two points along the line given by Eq. (B.3). Thus, Davidon's formulae are more elaborate and time consuming than those of Powell but Davidon's method ordinarily locates the minimum along the line in fewer iterations [91].

Each of the techniques previously listed will now be characterized with the steps of their algorithms being omitted. The details of the

algorithms are available in the appropriate literature cited.

B.2 Nelder-Mead's Simplex Method

In using the simplex method to minimize a function of N variables, the function is first evaluated at N + 1 mutually equidistant points in the space of the N variables. These points are called the vertices of a regular simplex which in two dimensions corresponds to an equilateral triangle and in three dimensions to a regular tetrahedron. This direct search technique using regular simplices was devised by Himsworth, Spendley and Hext [50]. Nelder-Mead's simplex method [53] represents an extension of their work wherein the regularity of the simplex is abandoned. Also, additional flexibility for adaptation of the simplex to the local geometry of the surface is incorporated. The basic operations of the simplex method are reflection, expansion and contraction. The vertex of the simplex with the highest function value is replaced by another point obtained through a reflection of that vertex. Depending on the value of the function at this new vertex, another reflection may be required or the simplex may expand or contract. These operations are repeated until the simplex essentially collapses on the minimum.

For each of these operations, a corresponding coefficient has been defined: a reflection coefficient α; a contraction coefficient β; and, an expansion coefficient γ. The values assigned to each of these coefficients are not fixed; however, Nelder and Mead's recommendation that the user set $\alpha = 1$, $\beta = 1/2$ and $\gamma = 2$ was

incorporated in this study. These values correspond to a simple reflection, halving when in difficulty and doubling when a useful direction is located.

One undesirable feature of the simplex method is that it requires a significant amount of computer storage when N is large. This is true because the coordinates of N + 1 vertices are stored throughout the minimization process.

B.3 Powell's Conjugate Direction Method

Another direct search method is the univariate method which seeks the minimum of a function of N variables by changing one variable at a time. The method of conjugate directions [56] is essentially a variation of the univariate method wherein the properties of a quadratic function are exploited. Neglecting the higher order terms, Eq. (B.2) is a quadratic function with a Hessian matrix $\underline{A}$ (i.e., $\frac{\partial^2 f}{\partial \underline{x}^2} = \underline{A}$). Search directions $\underline{d}_1, \ldots, \underline{d}_n \neq 0$ with the property

$$\underline{d}_i^T \underline{A} \underline{d}_j = 0, \quad i \neq j$$

are said to be conjugate or orthogonal with respect to the weighting matrix $\underline{A}$. Therefore, if these direction vectors are generated such that

$$\underline{d}_i = \underline{x}_i - \underline{x}_{i-1}$$

Then it can be shown [72,92] that they remain $\underline{A}$-conjugate and a conjugate direction has been defined.

In this technique, each iteration begins with a linear search along N linearly independent directions $\underline{d}_1$, $\underline{d}_2$, ..., $\underline{d}_N$, starting at the best known approximation to the location of the minimum. After an initial univariate search along each of the coordinate directions, conjugate directions are generated by making each iteration define a new search direction $\underline{d}$ and choosing $\underline{d}_2$, $\underline{d}_3$, ..., $\underline{d}_N$, $\underline{d}$ as the linearly independent directions for the next iteration. Applying this procedure to a positive definite quadratic form, all search directions will be mutually conjugate after N linear minimizations and the exact minimum will have been found. However, Powell modified his basic procedure because on occasions it may choose nearly dependent directions; particularly when minimizing a function of more than five independent variables [56,91]. To overcome this, he allows a direction other than $\underline{d}_1$ to be discarded. Therefore the N search directions can be chosen so as to be always linearly independent, even though, in some cases, the same N directions are used for two successive linear minimizations. As a consequence of this modification, one of the mutually conjugate directions may be discarded, thereby requiring more than N linear minimizations to find the exact minimum of a quadratic.

B.4 Method of Steepest Descent

The method of steepest descent, first proposed by Cauchy [60], is perhaps the oldest and most well known gradient technique for function minimization. It is based on moving in the opposite direction of the gradient vector for minimization. No other vector can locally

reduce the function value as much since the gradient vector perpen-
dicularly cuts adjacent contours of the function. While simple and
stable, this method often converges slowly and in a zig zag fashion.
This is because the direction of steepest descent and the direction to
the minimum may be nearly perpendicular [79]. Fletcher [48] attributes
this to the failure of the steepest descent theory to adequately repre-
sent functions with minima. He further asserts that "the only functions
for which the steepest descent property holds along the whole direction
of search and which still have a minimum are those with spherical con-
tours, and this does not adequately represent the minimum of a general
function" [48]. Research to strengthen this method for eccentric
functions or functions whose contours are distorted hyperspheres has
been carried out [93] but as Fox [92] points out, these modifications
are of little value when compared to more recent techniques for
function minimization.

B.5 Fletcher-Reeves' Conjugate Gradient Method

The conjugate gradient method is a special case of the more
general method of conjugate directions and was first developed by
Hestenes and Stiefel [63]. In the conjugate gradient method, the
search directions $\underline{d}_1$, ..., $\underline{d}_N$ are generated such that $\underline{d}_{i+1}$ represents
a linear combination of the present gradient vector g_{i+1} and previous
direction vectors $\underline{d}_1$, ..., $\underline{d}_i$. That is,

$$\underline{d}_{i+1} = -\underline{g}_{i+1} + \frac{g^2_{i+1}}{g^2_i} \underline{d}_i$$

With this scheme for defining new search directions, the property of these directions being A-conjugate is retained.

The Fletcher-Reeves algorithm [62] converts the N-dimensional problem into a sequence of one-dimensional problems; however, the accuracy of the one-dimensional minimization is not as crucial for this method as it is for the Davidon-Fletcher-Powell algorithm [45]. For quadratic functions, Myers [72] has shown that the direction vectors generated by the Fletcher-Reeves method are the same theoretically as those generated by the Davidon-Fletcher-Powell method, provided that the initial step for each method is taken in the direction of the steepest descent. This method reduces the convergence difficulties encountered by the method of steepest descent. Thus, accelerated convergence can be attained by reinitializing the search directions to those of the steepest descent method after every N + 2 iterations. This becomes especially necessary for nonquadratic functions because the conjugate gradient technique tends to generate nearly dependent search directions after N or so iterations [45]. With regard to reinitialization, Fox proposes that if the function is not both highly eccentric and twisted and "if the starting point is known to be a poor approximation to the minimum of a nonquadratic function, it may pay to restart after the first N or so cycles should they fail to produce a minimum, but not restart thereafter" [92].

B.6 Jacobson-Oksman's Method

The Jacobson-Oksman method [67] of function minimization is an

innovative and relatively new approach which is based not on quadratic functions of the type

$$f(\underline{x}) = \frac{1}{2}(\underline{x} - \underline{x}_m)^T \underline{A}(\underline{x} - \underline{x}_m) + \bar{\omega}$$

but on homogeneous functions of the form

$$f(\underline{x}) = \frac{1}{\gamma}(\underline{x} - \underline{x}_m)^T \underline{g}(\underline{x}) + \bar{\omega}$$

where

$\underline{A}$ is an N x N constant positive definite matrix

$\underline{x}_m$ is the location of the minimum

$\bar{\omega}$ is the minimum function value, $f(\underline{x}_m)$

γ is the degree of homogeneity.

Based on homogeneous functions, this algorithm is not concerned with either the Hessian matrix or approximations to its inverse. The method converges in N + 2 steps for homogeneous functions. However, only descent and not convergence has been proven for general functions. Therefore, the algorithm cannot be expected to converge in N + 2 steps for general functions. It is noteworthy to underscore the arduous task of programming the algorithm even though it requires neither the Hessian matrix nor a one-dimensional minimization scheme except to guarantee descent or stability.

B.7 Davidon-Fletcher-Powell's Variable Metric Method

Based on the original work of Davidon [71], Fletcher and Powell

modified the variable metric method in order to exploit its quadratic

convergence properties and its stability [77]. The essence of the

method is in the formation of a sequence of positive definite matrices

which are used in the determination of the search directions. Any

positive definite matrix may be used to start the iteration. This

matrix is then updated at each iteration and converges to the inverse

of the Hessian matrix at the minimum. The variable metric method also

replaces the N-dimensional minimization problem with a sequence of one-

dimensional minimizations using Davidon's cubic interpolation method.

Since gradient information is required for the variable metric method,

Stewart [78] has developed another modification allowing gradients

to be calculated by the finite difference technique if analytic

gradients are unavailable. Based on the fact that an approximation

to the inverse of the Hessian matrix is available, Stewart's modification

extracts an approximation to the Hessian matrix which is used to compute

the step size that will produce maximum accuracy in the finite dif-

ference gradient.

B.8 Davidon's Variance Method

Davidon's variance method [87], occasionally referred to as

Davidon's second method, is a similar yet simpler minimization

algorithm than his first method, the variable metric method [71].

Within this context, the term variance has been generalized to mean

the inverse of the Hessian matrix of any function, which will be

computed by successive estimates as in the original variable metric

algorithm. Therefore, the problem of inverting the Hessian matrix is avoided. Also, the one-dimensional minimization subproblem is no longer required provided a decrease in the function is realized at least once every N iterations [45]. However, the algorithm's principal drawback is its sensitivity to the user's selection of three parameters α, β and κ where $0 < \alpha < 1 < \beta$ and $\kappa > 0$ [45,87]. These parameters appear to be very much problem dependent and thereby limit the usefulness of this technique.

B.9 Fletcher's New Variable Metric Method

Derived from Davidon-Fletcher-Powell's variable metric algorithm, Fletcher's new variable metric method [81] dispenses with the linear search which is crucial to the Davidon-Fletcher-Powell algorithm and provides a new updating formula for the approximation to the inverse of the Hessian matrix. Having discarded the linear search, the property of quadratic termination cannot be proven and is replaced by a property for quadratic functions requiring that the eigenvalues of the inverse of the Hessian approximation tend monotonically toward those of the inverse of the Hessian matrix. Also required at each iteration is a sufficiently large reduction in the function value in order to guarantee ultimate convergence. An addition to the algorithm is the retention of the linear search capability which is invoked when it is necessary for other reasons to use more than one evaluation of the function and gradient per iteration.

APPENDIX C

DEVELOPMENT OF AN ANALYTIC GRADIENT
FOR FRAME ELEMENTS

The development of an analytic gradient of the functional S
wherein only geometric nonlinearities are included presents no in-
surmountable problem provided that the transformations from the local
coordinate system to the global coordinate system are correctly
implemented in the differentiation process. The derivative of the
i-th degree of freedom of the functional S of Eq. (1) can be expressed
as

$$
\frac{\partial S}{\partial X_{ei}} = M_i \left[\frac{6}{(\Delta t)^2} (X_{ei} - X_{oi}) - \frac{6}{(\Delta t)} \dot{X}_{oi} - 2\ddot{X}_{oi} \right]
$$

$$
- F_i \Big|_{t_o + \Delta t} + \frac{\partial U}{\partial X_{ei}} \tag{C.1}
$$

wherein X_{ei} is the i-th global generalized displacement. With the
exception of the last term in Eq. (C.1), the gradient calculation is
straightforward. The last term must be handled carefully as it
embraces the transformations from the local to the global coordinate
system. This derivative can be calculated as follows

$$
\frac{\partial U}{\partial X_{ei}} = \sum_{k=1}^{m} \frac{\partial U_k}{\partial X_{ei}} = \sum_{k=1}^{m} \sum_{j=1}^{6} \left(\frac{\partial U_k}{\partial q_j} \right) \left(\frac{\partial q_j}{\partial X_{ei}} \right) \tag{C.2}
$$

where q_j are the local generalized displacements and U_k is the strain
energy of the k-th element, k = 1, 2, ...,m with m being the number

of all such elements whose strain energies are affected by a change in the degree of freedom X_{ei}.

Since all the problems considered in this study involve only frame elements the development of the analytic gradient will be restricted to such elements only. The frame element is considered as a structural component that is initially straight and which undergoes axial, bending and torsional deformations resulting from finite displacements and rotations of its ends. Thus for the elastic case each element can have at most twelve degrees of freedom; six at each end.

The term $\dfrac{\partial U_k}{\partial q_j}$ of Eq. (C.2) can be readily expressed for the elastic case since a closed form expression for the elastic strain energy can be obtained. Neglecting the effects of shear, the following form can be easily derived

$$U_k = \frac{EL}{2}\left\{\left(\frac{\delta u}{L}\right)^2 A + \frac{12}{L^2}\left\{I_z\left[\left(\frac{\delta v}{L}\right)^2 - \left(\frac{\delta v}{L}\right)\psi_z + \frac{1}{3}\psi_z^2\right]\right.\right.$$

$$+ I_y\left[\left(\frac{\delta w}{L}\right)^2 + \left(\frac{\delta w}{L}\right)\psi_y + \frac{1}{3}\psi_y^2\right]$$

$$+ 2I_{yz}\left[\left(\frac{\delta v}{L}\right)\left(\frac{\delta w}{L}\right) + \frac{1}{2}\left(\frac{\delta v}{L}\right)\psi_y - \frac{1}{2}\left(\frac{\delta w}{L}\right)\psi_z\right.$$

$$\left.\left.\left.- \frac{1}{3}\psi_y\,\psi_z\right]\right\}\right\} \tag{C.3}$$

where

$$A = \int_A dA; \quad I_z = \int_A y^2\,dA$$

$$I_y = \int_A z^2\,dA; \quad I_{yz} = \int_A yz\,dA$$

E is the modulus of elasticity

L is the length of the element.

Also δu, δv, δw, ψ_x, ψ_y, ψ_z are the relative generalized displacements of the element. Therefore, the derivatives with respect to these variables, taking into account their equidimensionality, are as follows

$$\frac{\partial U_k}{\partial(\delta u)} = EA\left(\frac{\delta u}{L}\right)$$

$$\frac{\partial U_k}{\partial(\delta v)} = \frac{6E}{L^2}\left\{I_z\left[2\left(\frac{\delta v}{L}\right) - \psi_z\right] + 2\,I_{yz}\left[\left(\frac{\delta w}{L}\right) + \frac{1}{2}\psi_y\right]\right\}$$

$$\frac{\partial U_k}{\partial(\delta w)} = \frac{6E}{L^2}\left\{I_y\left[2\left(\frac{\delta w}{L}\right) + \psi_y\right] + 2\,I_{yz}\left[\left(\frac{\delta v}{L}\right) - \frac{1}{2}\psi_z\right]\right\}$$

$$\frac{\partial U_k}{\partial\psi_x} = 0$$

$$\frac{\partial U_k}{\partial\psi_y} = \frac{6E}{L^2}\left\{I_y\left[\left(\frac{\delta w}{L}\right) + \frac{2}{3}\psi_y\right]\right.$$
$$\left. + 2\,I_{yz}\left[\frac{1}{2}\left(\frac{\delta v}{L}\right) - \frac{1}{3}\psi_z\right]\right\}$$

$$\frac{\partial U_k}{\partial\psi_z} = \frac{6E}{L^2}\left\{I_z\left[-\left(\frac{\delta v}{L}\right) + \frac{2}{3}\psi_z\right]\right.$$
$$\left. - 2\,I_{yz}\left[\frac{1}{2}\left(\frac{\delta w}{L}\right) + \frac{1}{3}\psi_y\right]\right\}$$

The remaining term $\left(\frac{\partial q_j}{\partial X_{ei}}\right)$ can be thought of as a matrix which transforms a local gradient vector into a global gradient vector. In

order to derive this matrix, the deformed geometry of the frame element

needs to be discussed and will follow that given in reference [99].

Figure C.1 gives the initial position of a typical frame element

specified by the coordinates of its end points, the p and q joints it

connects, with respect to a fixed system of global coordinate axes

X, Y and Z. The longitudinal axis of the element and two reference

axes of the cross section, all mutually orthogonal, form the member

coordinate axes x_1, y_1 and z_1. A vector in the global coordinate

system can be described with respect to the member coordinate system

through an orthogonal transformation matrix. This transformation

matrix, $[T_1]$, describes large angular rotations from the global

coordinate axes X, Y, Z to the member coordinate axes x_1, y_1, z_1

and is given by Kamat et. al. [99] as

$$[T_1] = \begin{bmatrix} c_y \, c_z & c_y \, s_z & -s_y \\ -c_x \, s_z + s_x \, s_y \, c_z & c_x \, c_z + s_x \, s_y \, s_z & s_x \, c_y \\ s_x \, s_z + c_x \, s_y \, c_z & -s_x \, c_z + c_x \, s_y \, s_z & c_x \, c_y \end{bmatrix} \qquad (C.4)$$

where $c_i = \cos \phi_i$ and $s_i = \sin \phi_i$ for $i = x, y, z$. Angles ϕ_x, ϕ_y, ϕ_z

are defined in Figure C.1 and the rotations have been performed in the

order ϕ_z, ϕ_y and ϕ_x.

Motion of the frame element is a function of three translational

displacements and three rotational displacements of the two joints

which the member connects. To define joint displacements and

rotations, a set of joint axes are introduced at the joint p which are
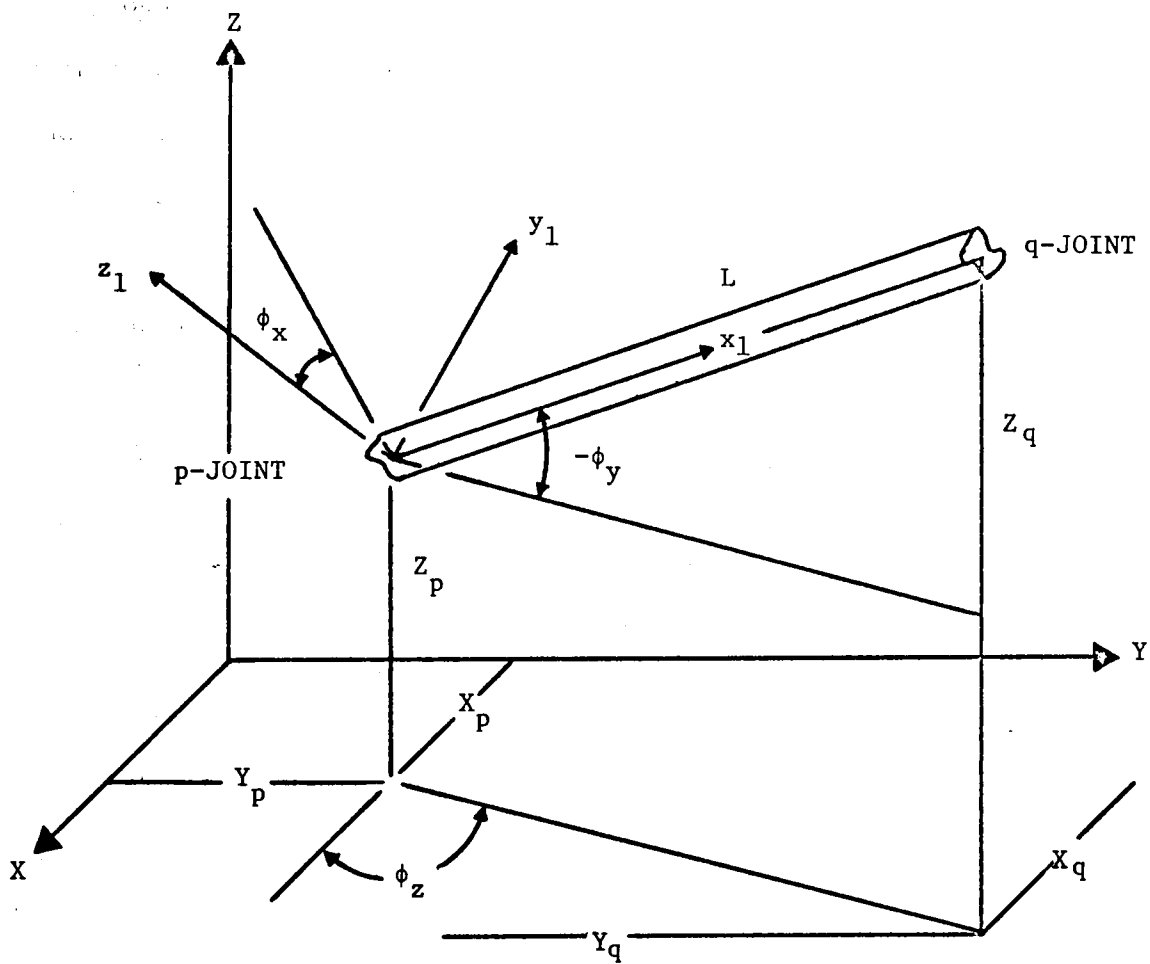
Figure C.1   Initial Geometry of the Frame Element
(Reproduced from Reference 99).

initially parallel to the global axes X, Y, Z. The joint displacements
are denoted by the vector $\underline{U}$ which has components U, V and W in the
X, Y and Z coordinate directions, respectively. The rotations of the
joint p, Θ_x, Θ_y, Θ_z, are about the joint axes which are parallel to
the global axes. Motion of the element is, thus, separated into two
parts: a rigid body motion which is described by the displacements
and rotations of joint p; and, a deformation which is described by
the motion of joint q relative to joint p.

Initially the joint axes are situated parallel to the global axes
with the origin at joint p. The rigid body motion translates and
rotates the joint axes to the position x', y', z' as shown in Figure
C.2. The translation is given by the vector $\underline{U}_p$ and the rotation is
described by the transformation matrix $[T_2]_p$ which relates vectors
in the global system to vectors in the displaced x', y', z' position
of the axes. The transformation matrix $[T_2]_p$ is identical in form
to $[T_1]$ of Eq. (C.1) except that the angles Θ_{xp}, Θ_{yp}, Θ_{zp} are used in
place of ϕ_x, ϕ_y, ϕ_z. The rotations must be specified in the order
Θ_{zp}, Θ_{yp}, Θ_{xp} to be able to use a form for $[T_2]_p$ similar to $[T_1]$. The
member axes remain fixed with respect to the joint axes. Rigid body
motion carries the joint axes from their initial position (parallel
to the global axes) to the position x', y', z'. Likewise, the member
axes x_1, y_1, z_1 become axes x_2, y_2, z_2 after the rigid body motion.
However, the new member axes x_2, y_2, z_2 are oriented exactly in the
same manner with respect to the joint axes x', y', z' as were the
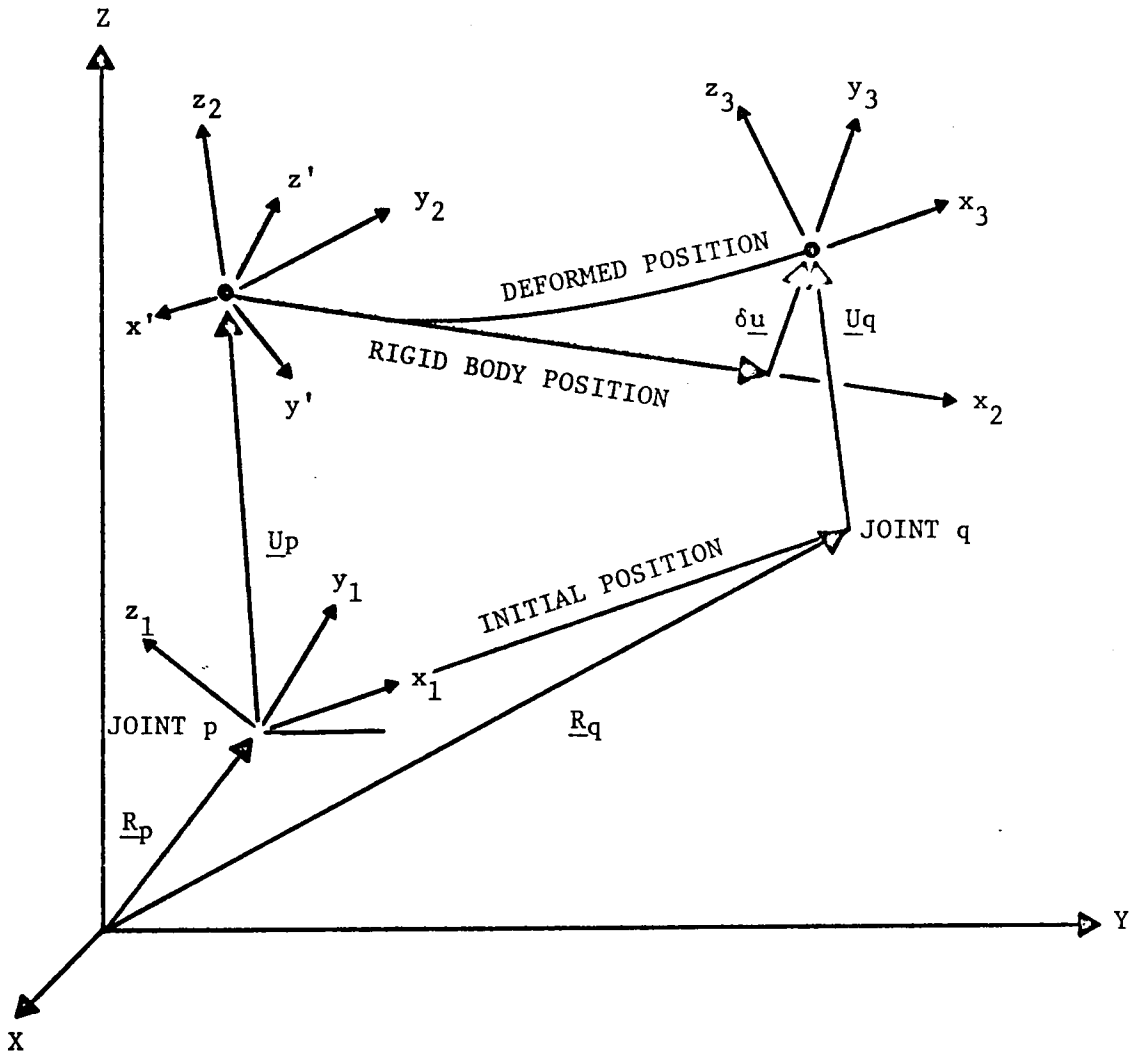member axes x_1, y_1, z_1 with respect to the global axes.

Figure C.2 Frame Element Motion (Reproduced from Reference 99).

To describe the deformation of the element, the displacements of the joint q need to be expressed with respect to the deformation axes. From Figure C.2, it follows that

$$\delta \underline{u} = (\underline{R}_q - \underline{R}_p) - \underline{L} + (\underline{U}_q - \underline{U}_p)$$

where $\delta \underline{u}$ is a vector described with respect to the deformation axes. Therefore,

$$
\begin{Bmatrix} \delta u \\ \delta v \\ \delta w \end{Bmatrix}
= [T_1] \left[[T_2]_p \begin{Bmatrix} \Delta X + \Delta U \\ \Delta Y + \Delta V \\ \Delta Z + \Delta W \end{Bmatrix} - \begin{Bmatrix} \Delta X \\ \Delta Y \\ \Delta Z \end{Bmatrix} \right]
\tag{C.5}
$$

where Δ is a difference operator for q and p end values in the global axes.

To complete the description of the deformation, expressions for the rotation of joint q with respect to the deformation axes are required. In the development of these expressions, the rotations of each joint are permitted to be large but the differences between the rotations defined by

$$\Delta\Theta_x = \Theta_{xq} - \Theta_{xp}; \quad \Delta\Theta_y = \Theta_{yz} - \Theta_{yp}; \quad \Delta\Theta_z = \Theta_{zq} - \Theta_{zp}$$

are assumed to be small, so that $\cos \Delta\Theta \simeq 1$ and $\sin \Delta\Theta \simeq \Delta\Theta$. By so doing, large rigid body motion of the element is allowed but the deformation of the element is restricted to small rotations. With this restriction, the small rotations ψ_x, ψ_y, ψ_z of joint q with respect to the deformation axes are given by

$$\left\{ \begin{array}{c} \psi_x \\ \psi_y \\ \psi_z \end{array} \right\} = [T_1] \ [T_2]_p \left\{ \begin{array}{c} \Delta\Theta_x \\ \Delta\Theta_y \\ \Delta\Theta_z \end{array} \right\} \tag{C.6}$$

Thus, deformation of the frame element is specified by the relative displacements and rotations of joint q with respect to joint p. Where the parameters δu, δv, δw, ψ_x, ψ_y, ψ_z are the generalized displacements as seen at joint q relative to joint p.

Two cases now need to be considered: (i) the geometrically linear case and (ii) the geometrically nonlinear case. Based on the convected coordinate formulation [96,99-104], the geometric nonlinearity arises entirely from the transformation from the local coordinate system to the global coordinate system. Therefore to include the effects of geometric nonlinearities, the large angle transformations, like Eq. (C.4), must be used for $[T_2]_p$ in Eq. (C.5) and (C.6). However, if displacements and rotations are constrained to be small and geometrically linear, approximate transformations may be employed by replacing the trigonometric functions by their power series expansion and retaining only the first order terms of the transformation. Thus, the resulting approximate transformations can be rewritten as

$$\{\delta u\} = \left\{ \begin{array}{c} \delta u \\ \delta v \\ \delta w \end{array} \right\} = [T_1] \left(\begin{bmatrix} 1 & \Theta_z & -\Theta_y \\ -\Theta_z & 1 & \Theta_x \\ \Theta_y & -\Theta_x & 1 \end{bmatrix} \left\{ \begin{array}{c} \Delta X \\ \Delta Y \\ \Delta Z \end{array} \right\} + \left\{ \begin{array}{c} \Delta U - \Delta X \\ \Delta V - \Delta Y \\ \Delta W - \Delta Z \end{array} \right\} \right) \tag{C.7}$$

$$\{\psi\} = \begin{Bmatrix} \psi_x \\ \psi_y \\ \psi_z \end{Bmatrix} = [T_1] \begin{Bmatrix} \Delta\Theta_x \\ \Delta\Theta_y \\ \Delta\Theta_z \end{Bmatrix} \tag{C.8}$$

Therefore, the gradient at each end of an element can be expressed as

$$\left(\frac{\partial U}{\partial X_{ei}}\right)_{p \text{ or } q} = \sum_{j=1}^{6} \left\{ \frac{\partial U}{\partial q_j} \left(\frac{\partial q_j}{\partial X_{ei}}\right)_{p \text{ or } q} \right\} \tag{C.9}$$

For the geometrically linear case, using Eq. (C.7) and (C.8),

$$\frac{\partial\{\delta u\}}{\partial\{U\}_p} = -[T_1]^T$$

$$\frac{\partial\{\delta u\}}{\partial\{U\}_q} = [T_1]^T$$

$$\frac{\partial\{\delta u\}}{\partial\{\Theta\}_p} = \begin{bmatrix} 0 & -\Delta Z & \Delta Y \\ \Delta Z & 0 & -\Delta X \\ -\Delta Y & \Delta X & 0 \end{bmatrix}^T [T_1]^T$$

$$\frac{\partial\{\delta u\}}{\partial\{\Theta\}_q} = [0]$$

$$\frac{\partial\{\psi\}}{\partial\{U\}_p} = [0]$$

$$\frac{\partial\{\psi\}}{\partial\{U\}_q} = [0]$$

$$\frac{\partial\{\psi\}}{\partial\{\Theta\}_p} = -[T_1]^T$$

$$\frac{\partial\{\psi\}}{\partial\{\Theta\}_q} = [T_1]^T$$

For the geometrically nonlinear case, using Eq. (C.5) and (C.6),

$$\frac{\partial\{\delta u\}}{\partial\{U\}_p} = -[T_2]_p^T [T_1]^T$$

$$\frac{\partial\{\delta u\}}{\partial\{U\}_q} = [T_2]_p^T [T_1]^T$$

$$\frac{\partial\{\delta u\}}{\partial\{\Theta\}_p} = [T_T]_p^T [T_1]^T$$

$$\frac{\partial\{\delta u\}}{\partial\{\Theta\}_q} = [0]$$

$$\frac{\partial\{\psi\}}{\partial\{U\}_p} = [0]$$

$$\frac{\partial\{\psi\}}{\partial\{U\}_q} = [0]$$

$$\frac{\partial\{\psi\}}{\partial\{\Theta\}_p} = [T_R]_p^T [T_1]^T$$

$$\frac{\partial\{\psi\}}{\partial\{\Theta\}_q} = [T_2]^T [T_1]^T$$

where the components of $[T_T]_p$ are

$$T_T^{11} = 0$$

$$T_T^{21} = (s_x s_z + c_x s_y c_z)(\Delta X + \Delta U) + (-s_x c_z$$

$$+ c_x s_y s_z)(\Delta Y + \Delta V) + c_x c_y(\Delta Z + \Delta W)$$

$$T_T^{31} = (c_x s_z - s_x s_y c_z)(\Delta X + \Delta U) - (c_x c_z$$

$$+ s_x s_y s_z)(\Delta Y + \Delta V) - s_x s_y(\Delta Z + \Delta W)$$

$$T_T^{12} = - s_y \, c_z (\Delta X + \Delta U) - s_y \, s_z (\Delta Y + \Delta V)$$

$$- c_y (\Delta Z + \Delta W)$$

$$T_T^{22} = s_x \, c_y \, c_z (\Delta X + \Delta U) + s_x \, c_y \, s_z (\Delta Y + \Delta V)$$

$$- s_x \, s_y (\Delta Z + \Delta W)$$

$$T_T^{32} = c_x \, c_y \, c_z (\Delta X + \Delta U) + c_x \, c_y \, s_z (\Delta Y + \Delta V)$$

$$- c_x \, s_y (\Delta Z + \Delta W)$$

$$T_T^{13} = - c_y \, s_z (\Delta X + \Delta U) + c_y \, c_z (\Delta Y + \Delta V)$$

$$T_T^{23} = (-c_x \, c_z - s_x \, s_y \, s_z)(\Delta X + \Delta U) + (-c_x \, s_z$$

$$+ s_x \, s_y \, c_z)(\Delta Y + \Delta V)$$

$$T_T^{33} = (s_x \, c_z - c_x \, s_y \, s_z)(\Delta X + \Delta U) + (s_x \, s_z$$

$$+ c_x \, s_y \, c_z)(\Delta Y + \Delta V)$$

and the components of $[T_R]_p$ are

$$T_R^{11} = - c_y \, c_z$$

$$T_R^{21} = (s_x \, s_z + c_x \, s_y \, c_z) \, \Delta\Theta_x - (-c_x \, s_z$$

$$+ s_x \, s_y \, c_z) + (-s_x \, c_z + c_x \, s_y \, s_z) \, \Delta\Theta_y$$

$$+ c_x \, c_y \, \Delta\Theta_z$$

$$T_R^{31} = (c_x \, s_z - s_x \, s_y \, c_z) \, \Delta\Theta_x - (s_x \, s_z + c_x \, s_y \, c_z)$$

$$- (c_x c_z + s_x s_y s_z) \Delta\Theta_y - s_x c_y \Delta\Theta_z$$

$$T_R^{12} = - s_y c_z \Delta\Theta_x - s_y s_z \Delta\Theta_y - c_y s_z$$

$$- c_y \Delta\Theta_z$$

$$T_R^{22} = s_x c_y c_z \Delta\Theta_x + s_x c_y s_z \Delta\Theta_y$$

$$- (c_x c_z + s_x s_y s_z) - s_x s_y \Delta\Theta_z$$

$$T_R^{32} = c_x c_y c_z \Delta\Theta_x + c_x c_y s_z \Delta\Theta_y$$

$$- (- s_x c_z + c_x s_y s_z) - c_x s_y \Delta\Theta_z$$

$$T_R^{13} = - c_y s_z \Delta\Theta_x + c_y c_z \Delta\Theta_y + s_y$$

$$T_R^{23} = (- c_x c_z - s_x s_y s_z) \Delta\Theta_x + (- c_x s_z$$

$$+ s_x s_y c_z) \Delta\Theta_y - s_x c_y$$

$$T_R^{33} = (s_x c_z - c_x s_y s_z) \Delta\Theta_x + (s_x s_z$$

$$+ c_x s_y c_z) \Delta\Theta_y - c_x c_y$$

Therefore, all terms in Eq. (C.2) have now been defined and the global gradient, Eq. (C.1), can be computed for an elastic analysis.

For the inelastic case, the calculational effect required per gradient calculation increases significantly compared to that of the elastic case. This results from the fact that stresses, strains and strain energies may vary over the volume of the element in a complex manner dependent on the material model. Hence the term $\frac{\partial U_k}{\partial q_j}$ must be

expressed in an alternate form such as

$$\frac{\partial U_k}{\partial q_j} = \int_{V_k} \left[\left(\frac{\partial W_k}{\partial \varepsilon_k} \right) \left(\frac{\partial \varepsilon_k}{\partial q_j} \right) \right] dV_k \qquad (C.10)$$

where W_k, ε_k and V_k are the strain energy density, the axial strain and the volume of the k-th element, respectively. Also, $\dfrac{\partial W_k}{\partial \varepsilon_k}$ is a stress-like quantity and $\dfrac{\partial \varepsilon_k}{\partial q_k}$ is the j-th component of the gradient vector of the axial strain for the k-th element.

The stress-like term is obtained by differentiating the expression for the strain energy density of the k-th element under the material's stress-strain curve, Figure C.3. Thus, it can be very easily shown for both one step incremental loading or unloading that

$$\left(\frac{\partial W_k}{\partial \varepsilon_k} \right) = \sigma_k$$

Next consider the gradient vector of the axial strain. It has been shown [105] that the linear axial displacement field of the elastic case has to be replaced by a quadratic variation of the axial
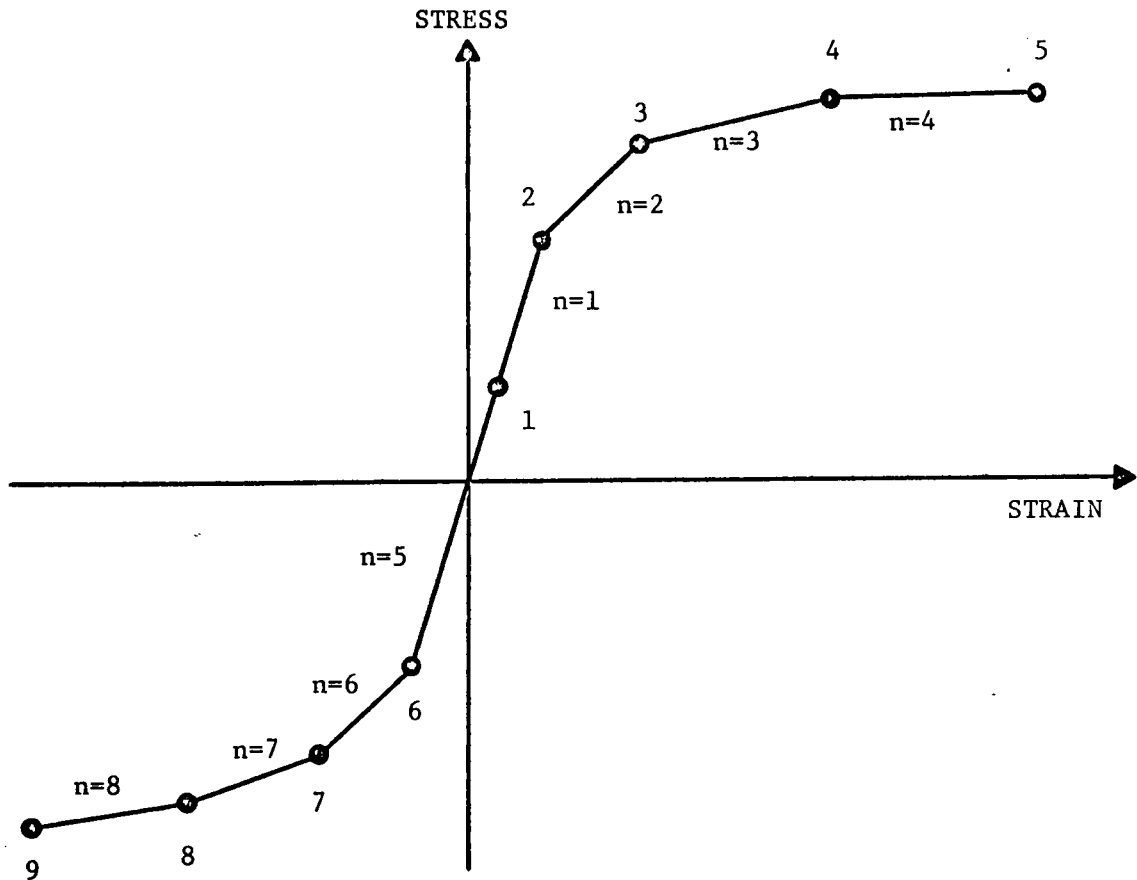
Figure C.3 Representation of the Stress-Strain Curve
(Reproduced from Reference 99).

displacement along the length of the element in order to satisfy equilibrium for inelastic response if the centroidal axis is used as a reference axis. This is achieved by introducing an additional node r at the center of the frame element wherein only the axial displacement, U, of this node is monitored. Therefore for inelastic response, a three noded (p, q, r) frame element with a total of thirteen degrees of freedom is used. The expression for the axial strain, neglecting the effects of shear, can now be written as

$$\varepsilon_k = (3 - 4 \frac{x}{L}) \frac{\delta u_1}{L} + (4 \frac{x}{L} - 1) \frac{\delta u_2}{L}$$

$$- \frac{y}{L} \left[6(1 - 2 \frac{x}{L}) \frac{\delta v}{L} + 2(3 \frac{x}{L} - 1) \psi_z \right]$$

$$- \frac{z}{L} \left[6(1 - 2 \frac{x}{L}) \frac{\delta w}{L} - 2(3 \frac{x}{L} - 1) \psi_y \right]$$

where $\delta u_1 = u_r - u_p;$

$\delta u_2 = u_q - u_r;$

x,y,z   are the local coordinates within the element.

The components of the gradient vector of the axial strain are as follows

$$\frac{\partial \varepsilon_k}{\partial(\delta u_1)} = (3 - 4 \frac{x}{L})$$

$$\frac{\partial \varepsilon_k}{\partial(\delta u_2)} = (4 \frac{x}{L} - 1)$$

$$\frac{\partial \varepsilon_k}{\partial(\delta v)} = - \frac{6y}{L} (1 - 2 \frac{x}{L})$$

$$\frac{\partial \, \varepsilon_k}{\partial (\delta w)} = - \frac{6z}{L} \left(1 - 2 \frac{x}{L}\right)$$

$$\frac{\partial \varepsilon_k}{\partial \psi_x} = 0$$

$$\frac{\partial \varepsilon_k}{\partial \psi_y} = \frac{2z}{L} \left(3 \frac{x}{L} - 1\right)$$

$$\frac{\partial \varepsilon_k}{\partial \psi_z} = - \frac{2y}{L} \left(3 \frac{x}{L} - 1\right)$$

where the equidimensionality of the variables has been taken into account.

Thus, the terms of the integrand of Eq. (C.10) have now been derived. However, analytic evaluation of this integral is extremely difficult for inelastic analysis and a numerical quadrature scheme is used. The frame element selected for this study is the solid rectangular cross sectional element of Figure C.4. This cross section is subdivided into four equal strips, each with four integration points per end, and the integration process is performed strip by strip. Therefore, Eq. (C.10) can be rewritten as

$$\frac{\partial U_k}{\partial X_{ei}} \Bigg|_{\ell} = \frac{dtL}{32} \sum_{m=1}^{4} \sum_{n=1}^{4} \left\{ \left[\left(\frac{\partial W_k}{\partial \varepsilon_k}\right) \left(\frac{\partial \varepsilon_k}{\partial q_j}\right)_{\ell} \right]_p \right.$$

$$\left. + \left[\left(\frac{\partial W_k}{\partial \varepsilon_k}\right) \left(\frac{\partial \varepsilon_k}{\partial q_j}\right)_{\ell} \right]_q \right\}_{mn} \left(\frac{\partial q_j}{\partial X_{ei}}\right)_{\ell} \qquad (C.11)$$
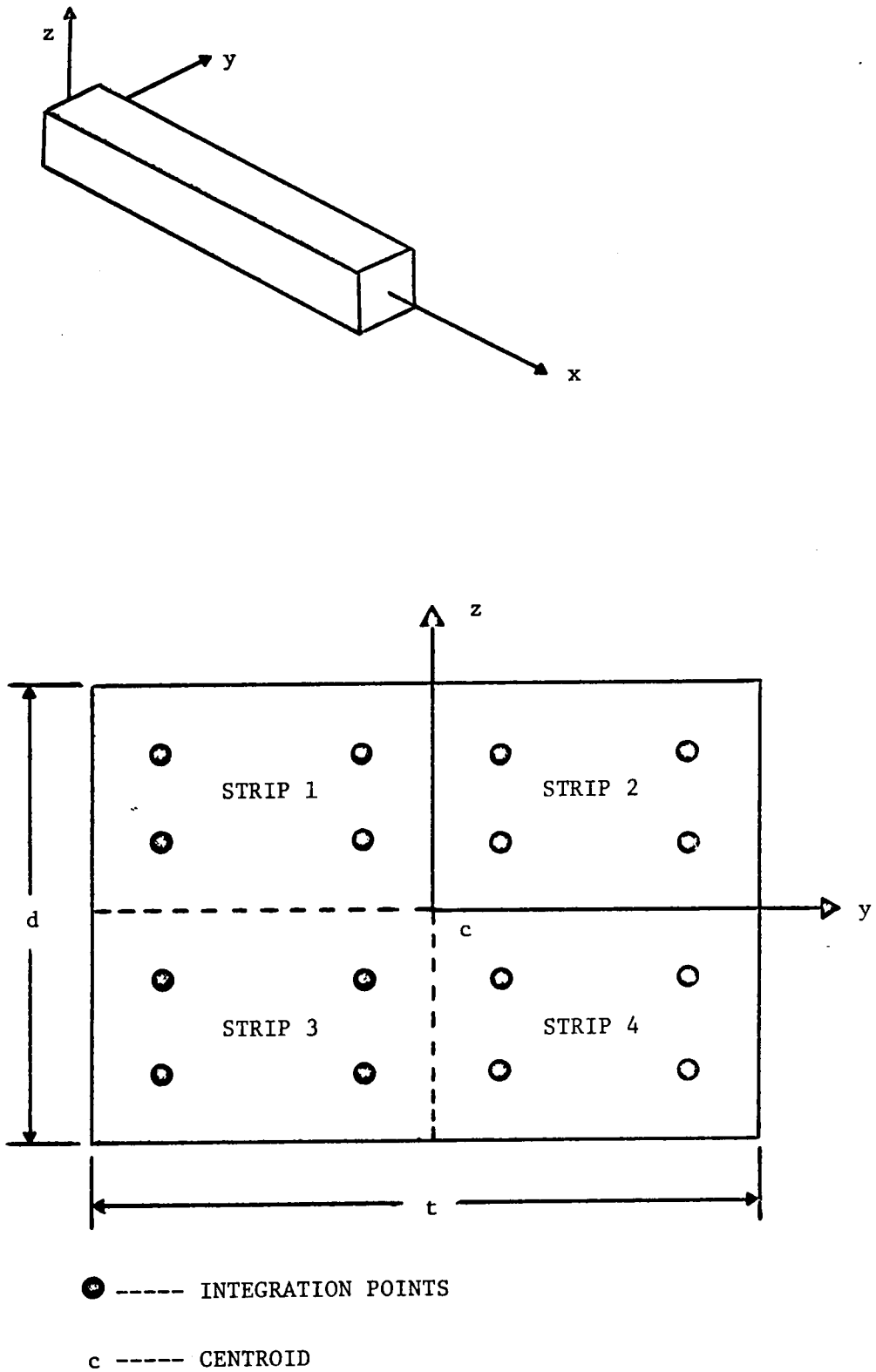
Figure C.4 Geometry of the Solid Rectangular Section

which represents the derivative of the strain energy U_k with respect to the i-th global degree of freedom X_{ei} at the ℓ-th node of the k-th member. The notation can be explained as follows: (i) the factor multiplying the summation results from a change in the limits of integration as required by the numerical quadrature scheme; (ii) the index m represents summation over the four strips of the element; (iii) the index n represents summation over the four integration points per end; (iv) the groups of terms inside the summation signs are similar and represent the product of the stress-like term and the gradient vector of the axial strain of the k-th member for the degrees of freedom at the ℓ-th node evaluated at both the p-end and the q-end; and, (v) the last term transforms the local gradient vector into a global gradient vector.

The transformations for the inelastic case are identical to those of the elastic case except for the transformation of the axial displacement terms. Recall that for the inelastic case, an additional node with only an axial degree of freedom was introduced at the center of the frame element. The development of the transformations of the axial displacement terms for the inelastic case follows, at least conceptually, that for the elastic case wherein the degree of freedom of the additional node is incorporated.

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AN EFFICIENCY ASSESSMENT OF SELECTED UNCONSTRAINED
MINIMIZATION TECHNIQUES AS APPLIED TO
NONLINEAR STRUCTURAL ANALYSIS

by

Norman F. Knight, Jr.

(ABSTRACT)

This thesis seeks to identify the potential for the uncon-
strained minimization algorithms of mathematical programming to be
cost-effective with the conventional techniques of nonlinear struc-
tural analysis. With this in mind, the author has attempted to
critically evaluate a few of the more commonly used algorithms for
their effectiveness in solving structural problems involving geo-
metric and/or material nonlinearities. The algorithms have been
categorized as being zeroth order requiring only function evalua-
tions, first order requiring evaluation of both the function and
the gradient or second order requiring in addition a variable
metric. The sensitivity of the first and second order algorithms
to the accuracy of derivatives derived on the basis of finite dif-
ference operations clearly suggests using analytically derived
derivatives in order to obtain better control of the computational
effort required for convergence to the exact solution. The thesis
concludes by attempting to identify the algorithm which promises

to be most effective in predicting nonlinear structural response and suggests improvements that could be made to make it even more cost-effective when compared with other well known techniques of nonlinear structural analysis.