

THE GRADIENT OF THE FINITE ELEMENT VARIATIONAL INDICATOR WITH RESPECT TO NODAL POINT CO-ORDINATES: AN EXPLICIT CALCULATION AND APPLICATIONS IN FRACTURE MECHANICS AND MESH OPTIMIZATION

THEODORE SUSSMAN[†] AND KLAUS-JÜRGEN BATHE[‡]
Massachusetts Institute of Technology, Cambridge, Massachusetts, U.S.A.

SUMMARY

We derive a closed-form expression for the change in the variational indicator of a finite element mesh with respect to perturbations in nodal point co-ordinates. The expression is evaluated very effectively from standard finite element data obtained in one solution, and may be easily programmed as part of a general finite element code. We present the derivation for two- and three-dimensional isoparametric elements used in linear and nonlinear elasticity. The expression has practical applications in the computation of stress intensity factors in fracture mechanics and in the determination of the 'optimal' mesh with a given element-node connectivity. We demonstrate both applications by accurately determining the stress intensity factor of a Mode I crack using a finite element mesh which was improved using mesh optimization.

INTRODUCTION

Problems in a variety of engineering disciplines can be solved using finite element procedures that operate on a variational indicator. This indicator, denoted by Π , is a scalar which can be computed for any possible solution of the problem and which has the property that Π is stationary for the exact solution.¹

In this paper we consider displacement-based finite element algorithms. These form approximate solutions by using displacement functions with unknown coefficients. The approximate solution is chosen by minimizing the variational indicator with respect to these coefficients. The finite element solution obtained depends on the mesh layout and on the locations of the nodal points; hence the variational indicator depends in the solution on the mesh layout and the nodal point co-ordinates.

In addition to the derivatives of Π with respect to the solution variables, the derivatives with respect to the nodal point co-ordinates of the finite element mesh can also be useful. Namely, the gradient of the variational indicator with respect to nodal co-ordinates can be used to solve problems of the form: 'If the nodal co-ordinates of a finite element representation are changed slightly while the loads are kept unchanged, what is the effect on the variational indicator?' We will describe two problems of this form below. Current solutions to these problems generally involve either specialized techniques or employ finite difference approximations to estimate the

[†] Research Assistant.

[‡] Professor of Mechanical Engineering.

gradient. In this paper we will present an explicit expression which can be used to efficiently evaluate the gradient of Π with respect to nodal co-ordinates.

One problem of the general form described above is the determination of the stress intensity factor of a cracked body. In many cases, the stress intensity factor may be calculated from the 'energy release rate' of the crack; this is the rate of change of the strain energy of the body as the crack tip advances.²

Currently, the energy release rate is frequently evaluated using finite element based techniques.³ Typical methods used include the compliance method, stiffness derivative method,^{4,5} J-integral method⁶ and deLorenzi's method.⁷ These methods incorporate one or more of the following undesirable features:

1. Finite difference approximations are used (compliance method, stiffness derivative method).
2. An arbitrary path for surface integration must be chosen (J-integral method).
3. The method can only be used to solve energy release rate problems and cannot be used to solve problems of the more general type described above (J-integral method, deLorenzi's method).

Since the strain energy is numerically equal to the negative of the variational indicator¹ and the crack geometry is described by nodal point co-ordinates, the problem of determining the energy release rate is a special case of the more general problem discussed above. Therefore, our expression for the gradient of Π with respect to nodal point co-ordinates may also be used to evaluate the energy release rate. Because the derivatives of Π are efficiently evaluated, this is a simple, effective method of finding the energy release rate.

Another problem of this general type is the problem of improving a finite element mesh using nodal point co-ordinate (NPC) optimization. Because the value of Π for the exact solution is unknown, but is less than Π for the finite element solution, it is desirable to minimize Π as much as possible to minimize the solution error. This is normally done by refining the mesh (adding more elements). Another approach is to choose nodal co-ordinates which minimize the variational indicator without changing either the element-node connectivity or the geometry of the body. We call the mesh with these co-ordinates 'optimal' and the process of determining this mesh is called nodal point co-ordinate (NPC) optimization. Note that unless the mesh is optimal, the variational indicator will change as nodal co-ordinates are changed (infinitesimally) even if the geometry of the body is unaffected.

Algorithms for NPC optimization have been studied by several researchers.^{8,9} Because the optimization problem is nonlinear, the basic approach used in NPC optimization is to improve an existing finite element mesh by shifting nodal co-ordinates and/or displacements using an iterative algorithm. This algorithm frequently requires the gradient of the variational indicator with respect to admissible nodal co-ordinate perturbations (in Reference 9, for example, this gradient is determined using finite difference approximations). However, using our explicit expression for the gradient of Π with respect to nodal co-ordinates can significantly improve the efficiency of NPC optimization algorithms.

In the next section we present the derivation of a closed-form expression giving the change in the variational indicator to perturbations in nodal co-ordinates. The expression is valid for three-dimensional isoparametric finite elements used in elasticity solutions. Expressions for two-dimensional plane stress, plane strain and axisymmetric elements are also presented. All of these expressions are numerically evaluated using calculated data from one finite element solution.

Next, we show how we can use our expression directly to calculate the energy release rate for a two-dimensional crack and we discuss how our expression may be used in NPC optimization. To demonstrate these applications, we present a simple example involving a two-dimensional

cracked specimen in Mode I loading. In the example, we modelled the specimen with four 8-node finite elements (deliberately not using special techniques to model the crack tip) and calculated the stress intensity factor. Then we improved the mesh using NPC optimization and recalculated the stress intensity factor. Because the improved mesh featured mid-side nodes nearest the crack tip at the quarter-points, the stress intensity factor improved markedly as a result of the NPC optimization.

DERIVATION OF AN EXPRESSION FOR THE CHANGE IN THE VARIATIONAL INDICATOR WITH RESPECT TO NODAL POINT CO-ORDINATES

As we discussed above, an explicit expression for the change in the variational indicator with respect to nodal point co-ordinate perturbations is useful in the fields of mesh optimization and in fracture mechanics. This section will present the derivation of the expression for three-dimensional isoparametric finite elements used in linear elasticity. The expression is then simplified for the special cases of two-dimensional plane stress, plane strain and axisymmetric problems.

Our procedure is based on the recognition of the fact that the discretized variational indicator Π depends on both the nodal point displacements u_i^n and on the nodal point co-ordinates x_i^n (the subscript refers to the direction and the superscript refers to the global node number). Furthermore, the nodal point co-ordinates can be varied independently of the nodal point displacements since the variational indicator is computable for all admissible combinations of coordinates and displacements. With this in mind, the change in the variational indicator can be written using a first-order Taylor series as[†]

$$d\Pi = \left(\frac{\partial \Pi}{\partial u_i^n} \right) du_i^n + \left(\frac{\partial \Pi}{\partial x_i^n} \right) dx_i^n \quad (1)$$

where each partial derivative is computed assuming that all other co-ordinates and displacements are fixed.

If the co-ordinates and displacements are chosen arbitrarily, $d\Pi$ is a function of both du_i^n and dx_i^n . However, if the u_i^n 's are chosen so as to make either $\partial \Pi / \partial u_i^n$ or du_i^n zero for each u_i^n , then $d\Pi$ will only be a function of the dx_i^n 's. Fortunately, the unique set of displacements with this property is the set of displacements chosen by finite element algorithms since these algorithms minimize Π with respect to nodal point displacements. In this case, equation (1) reduces to

$$d\Pi = \left(\frac{\partial \Pi}{\partial x_i^n} \right) dx_i^n \quad (2)$$

in which $\partial \Pi / \partial x_i^n$ is computed assuming that all nodal point displacements are fixed.

Before we expand equation (2), we illustrate the above argument. The variational indicator for linear elasticity may be written as¹

$$\Pi = \frac{1}{2} \mathbf{u}^T \mathbf{K} \mathbf{u} - \mathbf{R}^T \mathbf{u} \quad (3)$$

where \mathbf{u} is the displacement vector, \mathbf{K} is the stiffness matrix and \mathbf{R} is the nodal loads vector. In this equation, \mathbf{R} and \mathbf{K} depend on the nodal co-ordinates only. Now equation (1) can be written as

$$d\Pi = \left[\frac{1}{2} \mathbf{u}^T \frac{\partial \mathbf{K}}{\partial x_i^n} \mathbf{u} - \frac{\partial \mathbf{R}^T}{\partial x_i^n} \mathbf{u} \right] dx_i^n + \left[\left(\mathbf{K} \mathbf{u} - \mathbf{R} \right)^T \frac{\partial \mathbf{u}}{\partial u_i^n} \right] du_i^n \quad (4)$$

[†]Throughout the paper we use the usual indicial notation of summation convention.¹

However, finite element algorithms choose \mathbf{u} so that $\mathbf{Ku} - \mathbf{R} = \mathbf{0}$. Therefore

$$d\Pi = \left[\frac{1}{2} \mathbf{u}^T \frac{\partial \mathbf{K}}{\partial x_i^n} \mathbf{u} - \frac{\partial \mathbf{R}^T}{\partial x_i^n} \mathbf{u} \right] dx_i^n \tag{5}$$

which is in the same form as equation (2). Note that the term in brackets is the ‘stiffness derivative’ expression used in fracture mechanics.^{4,5}

Equation (5) is difficult to expand since $\partial \mathbf{K} / \partial x_i^n$ must be computed for each element of \mathbf{K} and each value of i and n . Therefore we do not use equation (3) for the variational indicator, but instead write the variational indicator as

$$\Pi = \mathcal{U} - \mathcal{W} \tag{6}$$

where \mathcal{U} is the sum of the element strain energies,

$$\mathcal{U} = \sum_{\text{elements}} \mathcal{U}^{(m)} = \sum_{\text{elements}} \int_V \frac{1}{2} \tau_{kl} \varepsilon_{kl} dV \tag{7}$$

and \mathcal{W} is the potential of the applied loads,

$$\mathcal{W} = R_k^p u_k^p + \sum_{\text{elements}} \mathcal{W}^{(m)} = R_k^p u_k^p + \sum_{\text{elements}} \int_S f_k^S u_k dS + \sum_{\text{elements}} \int_V f_k^B u_k dV \tag{8}$$

In these expressions, τ_{kl} is the stress tensor, ε_{kl} is the small strain tensor, R_k^p is an applied concentrated force on node p , f_k^S is an applied surface traction and f_k^B is an applied body force. Using these definitions, and noting that the concentrated forces R_k^p do not depend on the nodal co-ordinates, equation (2) becomes

$$d\Pi = \left[\sum_{\text{elements}} \left(\frac{\partial \mathcal{U}^{(m)}}{\partial x_i^n} \right) - \sum_{\text{elements}} \left(\frac{\partial \mathcal{W}^{(m)}}{\partial x_i^n} \right) \right] dx_i^n \tag{9}$$

We can now expand the partial derivatives using chain differentiation as shown below.

First we expand the strain energy term. Assuming that three-dimensional isoparametric elements are used, and assuming linear elasticity,

$$\mathcal{U}^{(m)} = \frac{1}{2} \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 \tau_{kl} \varepsilon_{kl} |\mathbf{J}| dr_1 dr_2 dr_3 \tag{10}$$

where the r_i , $i = 1, 2, 3$ are the isoparametric co-ordinates and $|\mathbf{J}|$ is the Jacobian determinant.¹ This can also be written as

$$\mathcal{U}^{(m)} = \frac{1}{2} \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 C_{klpq} u_{k,l} u_{p,q} |\mathbf{J}| dr_1 dr_2 dr_3 \tag{11}$$

where C_{klpq} is the constitutive constants tensor and where differentiation with respect to a co-ordinate direction is denoted by a comma.[†] Therefore, the partial derivative of $\mathcal{U}^{(m)}$ required in equation (9) is

$$\frac{\partial \mathcal{U}^{(m)}}{\partial x_i^n} = \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 \left(\tau_{kl} \frac{\partial u_{k,l}}{\partial x_i^n} |\mathbf{J}| + \frac{1}{2} \tau_{kl} \varepsilon_{kl} \frac{\partial |\mathbf{J}|}{\partial x_i^n} \right) dr_1 dr_2 dr_3 \tag{12}$$

To complete the expansion, we need to write the terms $u_{k,l}$ and $|\mathbf{J}|$ in a more explicit

[†]Note that $\partial / \partial x_i \neq \partial / \partial x_i^n$ because $\partial / \partial x_i$ represents a change with respect to a co-ordinate direction and $\partial / \partial x_i^n$ represents a change with respect to the nodal co-ordinate x_i^n .

form. We use

$$u_{k,1} = (\bar{\varepsilon}_{abc} u_{k,r_a} x_{2,r_b} x_{3,r_c}) / |\mathbf{J}| \quad (13a)$$

$$u_{k,2} = (\bar{\varepsilon}_{abc} x_{1,r_a} u_{k,r_b} x_{3,r_c}) / |\mathbf{J}| \quad (13b)$$

$$u_{k,3} = (\bar{\varepsilon}_{abc} x_{1,r_a} x_{2,r_b} u_{k,r_c}) / |\mathbf{J}| \quad (13c)$$

$$|\mathbf{J}| = \bar{\varepsilon}_{abc} x_{1,r_a} x_{2,r_b} x_{3,r_c} \quad (14)$$

where $\bar{\varepsilon}_{abc}$ is the permutation operator. Now the rest of the derivation for $\partial \mathcal{W}^{(m)} / \partial x_i^n$ is just chain differentiation which is summarized in Appendix I. The final result for $\partial \mathcal{W}^{(m)} / \partial x_i^n$ is

$$\frac{\partial \mathcal{W}^{(m)}}{\partial x_i^n} = \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 \left(\frac{1}{2} \tau_{pq} u_{p,q} h_{n,i} - \tau_{ki} u_{k,i} h_{n,i} \right) |\mathbf{J}| dr_1 dr_2 dr_3 \quad (15)$$

where h_n is the isoparametric interpolation function corresponding to node n . This completes the expansion of the strain energy derivative term.

We note that this expression is quite similar to deLorenzi's expression for the energy release rate at crack tips.

Next we use chain differentiation to expand $\partial \mathcal{W}^{(m)} / \partial x_i^n$. We find that

$$\begin{aligned} \frac{\partial \mathcal{W}^{(m)}}{\partial x_i^n} = & \sum_{\text{surfaces}} \left\{ \int_{-1}^1 \int_{-1}^1 (f_k^S u_k) [h_{n,s_2} (x_{i,s_2} E - x_{i,s_1} F) + h_{n,s_1} (x_{i,s_1} G - x_{i,s_2} F)] (EG \right. \\ & \left. - F^2)^{-1/2} ds_1 ds_2 \right\} + \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 f_k^B u_k h_{n,i} |\mathbf{J}| dr_1 dr_2 dr_3 \end{aligned} \quad (16)$$

where $E = x_{j,s_1} x_{j,s_1}$, $F = x_{j,s_1} x_{j,s_2}$, $G = x_{j,s_2} x_{j,s_2}$ and s_1, s_2 are the isoparametric co-ordinates over an element surface.

We note that, although equations (15) and (16) were derived for linear elasticity, the only modification required for nonlinear elasticity is to replace in equation (15) the term $\frac{1}{2} \tau_{pq} u_{p,q}$ with the actual strain energy density. This means that these equations may be used to solve deformation plasticity problems, since deformation plasticity is a special case of nonlinear elasticity.

Note that the expressions in equations (15) and (16) can be evaluated for given finite element co-ordinate and displacement data in a very effective way using the current stress and strain conditions and derivatives of the interpolation functions. Equations (9), (15) and (16), when combined, give the desired expression for the change in the variational indicator with respect to nodal co-ordinate perturbations.

The above derivation can be used to obtain the corresponding expressions for two-dimensional plane stress, plane strain and axisymmetric elements. Appendix II presents the derivations for these elements.

In practical analysis, numerical integration is used to evaluate the stiffness matrix and load vector. This effectively means that the integrals in equations (7) and (8) are replaced by summations. Similarly, the formulae given above are also evaluated using the numerical integration algorithms used in the finite element calculations.

APPLICATIONS OF THE GRADIENT OF Π WITH RESPECT TO NODAL CO-ORDINATES IN LINEAR ELASTICITY

In this section we discuss two applications for the explicit expression for the gradient derived in the last section. First, we discuss how this gradient is used to calculate stress intensity factors in fracture mechanics; then we discuss how this gradient is used in NPC optimization.

Calculation of energy release rates in fracture mechanics

In fracture mechanics, the energy release rate for a crack is defined by

$$G = \frac{-d\Pi}{dA} \quad (17)$$

where dA is the change in the crack area. Since this area is a function of the nodal point co-ordinates only, equation (17) can be written as

$$G = \frac{-\partial\Pi}{\partial x_i^n} \frac{\partial x_i^n}{\partial A} \quad (18)$$

Now, if $\partial x_i^n / \partial A$ is known for a crack geometry, then the expression derived in the last section for $\partial\Pi / \partial x_i^n$ may be used to calculate the energy release rate efficiently.

In two-dimensional plane stress or plane strain analyses, the crack tip is represented by a single node; therefore, the change in the crack area can be modelled by motions of that node. If a crack tip node is denoted by c , then

$$\begin{aligned} \frac{\partial x_i^n}{\partial A} &= 0 & n \neq c \\ \frac{\partial x_i^n}{\partial A} &= \frac{a_i}{t} & n = c \end{aligned} \quad (19)$$

where the a_i are the components of the unit vector in the direction of crack propagation and t is the specimen thickness. In theory, the unit vector could be chosen from the requirement that the crack tip will propagate in the direction which maximizes G ;¹⁰ however, we consider only problems in which the crack tip is known to propagate in the existing crack direction. Equation (17) then becomes

$$G_c = \frac{-\partial\Pi}{\partial x_i^n} \frac{a_i}{t} \quad (\text{no sum on } c) \quad (20)$$

where G_c is the energy release rate for the crack tip modelled with node c .

Equation (20) may be evaluated quite efficiently since only the gradient of Π with respect to node c is required. The cost of computing these derivatives is less than that needed to compute the finite difference approximations in the compliance and stiffness derivative methods. In addition, equation (20) avoids the disadvantage of having to evaluate a surface integral (as in the J-integral method). A comparison of deLorenzi's method with our method shows that the two methods are quite equivalent; but deLorenzi's equations are limited to stress intensity factor calculations because they were derived specifically for cracked bodies.

Nodal point co-ordinate optimization

The goal in NPC optimization is to produce an 'optimal' mesh; that is, a mesh in which Π is minimized with respect to all admissible nodal point co-ordinate perturbations as well as with respect to all admissible nodal point displacements. Because closed form solutions to the problem of selecting optimal nodal co-ordinates do not exist, the optimization algorithms are iterative.

Two options are available in mesh optimization. First, one could consider the co-ordinates and displacements as independent variables and, using an optimization algorithm, iterate on co-ordinates and displacements simultaneously until Π is minimized. This is the approach used

by Carpenter and Zendegui.⁹ The second approach is to iterate on just the co-ordinates, and after each iteration, to compute the displacements using standard finite element algorithms. Although this may be more expensive than the first approach, the second approach has the advantage that the optimization algorithm can be programmed as a post-processor for an existing finite element program. A discussion of a simple optimization algorithm based on this technique is given in our previous paper.¹³

Regardless of which option is used, our expression for the gradient of Π with respect to nodal co-ordinates is useful, since it allows the efficient use of optimization algorithms which operate on the gradient of the objective function, such as the BFGS method.¹ The only modifications which must be made to the partial derivatives produced by our formulae are the additions of the nodal restraints needed to prevent distortion of the structural geometry. These modifications are made node-by-node by only allowing nodal movements that do not violate the boundary conditions and that preserve the geometry of the body.

Example: a cracked specimen

To demonstrate the effectiveness of our expression, we consider the problem of determining the stress intensity factor K_I of the two-dimensional specimen shown in Figure 1. Assuming a plane strain solution, the stress intensity factor can be calculated using

$$K_I = \sqrt{\left(\frac{E}{1-\nu^2} G\right)} \quad (21)$$

where G is the energy release rate. For this specimen, the 'exact' value of the stress intensity factor (accurate to within 1 per cent) is $532 \text{ N/m}^{3/2}$ (Reference 11).

The specimen was analysed using the four 8-node element model shown in Figure 2. The finite element calculations were made using the program ADINA¹² and a Gauss integration order of

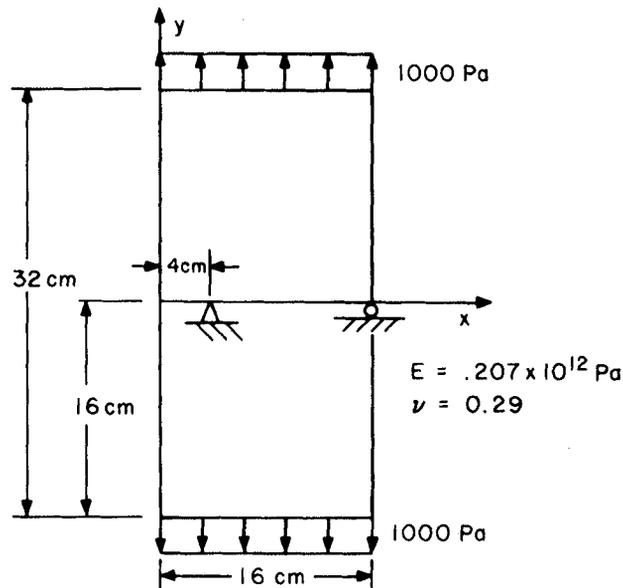


Figure 1. The cracked specimen considered, in plane strain; 'exact' stress intensity factor K_I is $532 \text{ N/m}^{3/2}$

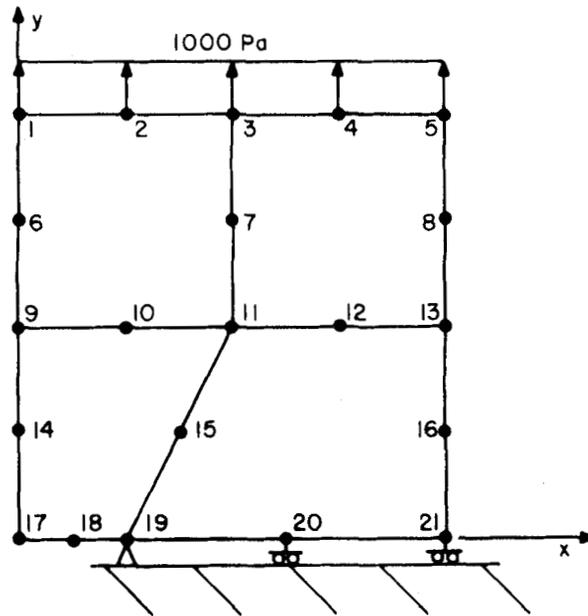


Figure 2. Four-element model of cracked specimen; calculated stress intensity factor K_I is $421 \text{ N/m}^{3/2}$

4 was used in all calculations. Note that no special consideration was given to the crack tip; no collapsed elements were used and all mid-side nodes were located at the element half-points.

Applying equation (20) in conjunction with our expression gave $G = 7.8318 \times 10^{-7} \text{ J/m}^2$; $K_I = 421 \text{ N/m}^{3/2}$. Only the crack tip node was used in modelling the crack advance. It is seen that the error is significant (about 20 per cent).

However, this error is mainly due to the poor choice of nodal point co-ordinates. We demonstrated this by improving the mesh using an NPC optimization algorithm. Our algorithm iterated

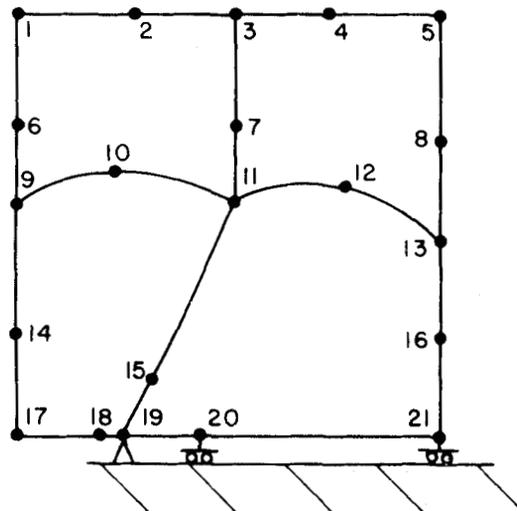


Figure 3. Optimal mesh for four-element model of cracked specimen; calculated stress intensity factor K_I is $523 \text{ N/m}^{3/2}$

on co-ordinates alone; ADINA was used to compute displacements and a post-processor generated the new trial meshes. Eighteen trial meshes were needed to generate the improved mesh shown in Figure 3 (but by far most of the improvement was obtained in the first six iterations). During the 18 iterations, the variational indicator decreased from $-6.2375 \times 10^{-8} \text{ J}$ to $-6.5768 \times 10^{-8} \text{ J}$ and the stress intensity factor increased from $421 \text{ N/m}^{-3/2}$ to $523 \text{ N/m}^{-3/2}$. The improvement in stress intensity factor can be explained by noting that the mid-side nodes nearest the crack tip moved to the quarter-points; this generated the $r^{-1/2}$ stress singularity at the crack tip.¹⁴

The following conclusions can be drawn from this example:

1. The stress intensity factor was accurately calculated (to within 2 per cent) using our closed-form expression for the partial derivatives of Π with respect to nodal co-ordinates.
2. NPC optimization produced a mesh with distorted elements with curved sides and mid-side nodes moved from the half-points.
3. In this example, we modelled the crack advance with the nodal movement of just the crack tip node. We could also have moved nearby nodes along with the crack tip node (to keep these nodes at the quarter-points, for example). However, as long as the motions of the nearby nodes do not affect the specimen geometry, the predicted value for the stress intensity factor is unchanged. This is a direct result of the NPC optimization process since Π was made stationary to any perturbation in nodal co-ordinates which did not affect the specimen geometry.

CONCLUSIONS

In this paper we have derived a closed-form expression for the change in the variational indicator Π with respect to the nodal point co-ordinates. The theory used in the derivation can be applied to all finite element problems possessing a variational indicator because the variational indicator can be computed from any admissible combination of nodal point co-ordinates and nodal point solution coefficients and because standard finite element algorithms choose nodal solution coefficients optimally. Therefore, although our expression is valid for isoparametric finite elements used in linear and nonlinear elasticity, corresponding formulae can be derived for other elements and for other classes of problems (such as heat transfer and field problems).

We demonstrated the usefulness of this expression in the fields of fracture mechanics and in NPC optimization. In fracture mechanics, the energy release rate (and therefore the stress intensity factor) can be efficiently computed using the partial derivatives in our expression. We note that our technique yields the same results as earlier methods; however, our method is very simple and efficient and may be easily programmed. Our treatment of this problem was limited to simple two-dimensional geometries and loadings; however, the basic principle can be extended to more complex problems. In NPC optimization, our formulae may be used to compute the gradient of Π with respect to admissible nodal motions without the expense of computing finite difference approximations. Both applications were demonstrated by an example, in which the stress intensity factor of a two-dimensional cracked specimen was accurately calculated using a four 8-node element model which had been improved using NPC optimization. Although the crack tip had not been specially modelled in the initial mesh (Figure 2), the mid-side nodes nearest the crack tip automatically moved to the quarter-points to create the $r^{-1/2}$ singularity (Figure 3). This example demonstrates that NPC optimization can be a powerful tool for the theoretical study of finite element meshes.

ACKNOWLEDGEMENTS

We gratefully acknowledge the fellowship provided earlier to T. Sussman by Bell Laboratories through their One Year On Campus program, and the support of ADINA Engineering for this work.

APPENDIX I: DERIVATION OF THE TERMS $\partial u_{k,l}/\partial x_i^n, \partial |\mathbf{J}|/\partial x_i^n$

The transformation between derivatives of u_k with respect to global co-ordinates and derivatives of u_k with respect to isoparametric co-ordinates is given by

$$u_{k,r_a} = x_{j,r_a} u_{k,j} \quad (22)$$

Since this is a system of linear simultaneous equations, Cramer's rule may be used to derive

$$u_{k,1} = (\bar{e}_{abc} u_{k,r_a} x_{2,r_b} x_{3,r_c}) / |\mathbf{J}| \quad (23a)$$

$$u_{k,2} = (\bar{e}_{abc} x_{1,r_a} u_{k,r_b} x_{3,r_c}) / |\mathbf{J}| \quad (23b)$$

$$u_{k,3} = (\bar{e}_{abc} x_{1,r_a} x_{2,r_b} u_{k,r_c}) / |\mathbf{J}| \quad (23c)$$

$$|\mathbf{J}| = \bar{e}_{abc} x_{1,r_a} x_{2,r_b} x_{3,r_c} \quad (24)$$

where \bar{e}_{abc} is the permutation operator. Now, using

$$x_{k,r_a} = h_{m,r_a} x_k^m \quad (25)$$

and

$$u_{k,r_a} = h_{m,r_a} u_k^m \quad (26)$$

where h_m is the function which interpolates the co-ordinates of global node m in the element considered, gives

$$d|\mathbf{J}| = \bar{e}_{abc} h_{m,r_a} x_{2,r_b} x_{3,r_c} dx_1^m + \bar{e}_{abc} x_{1,r_a} h_{m,r_b} x_{3,r_c} dx_2^m + \bar{e}_{abc} x_{1,r_a} x_{2,r_b} h_{m,r_c} dx_3^m \quad (27)$$

$$\begin{aligned} du_{k,1} = & -u_{k,1} |\mathbf{J}|^{-1} (\bar{e}_{abc} h_{m,r_a} x_{2,r_b} x_{3,r_c}) dx_1^m + |\mathbf{J}|^{-1} \bar{e}_{abc} (u_{k,r_a} h_{m,r_b} x_{3,r_c} - u_{k,1} x_{1,r_a} h_{m,r_b} x_{3,r_c}) dx_2^m \\ & + |\mathbf{J}|^{-1} \bar{e}_{abc} (u_{k,r_a} x_{2,r_b} h_{m,r_c} - u_{k,1} x_{1,r_a} x_{2,r_b} h_{m,r_c}) dx_3^m \end{aligned} \quad (28)$$

with similar terms for $du_{k,2}$ and $du_{k,3}$. The partial derivatives of these terms with respect to a nodal co-ordinate are found by assuming that only the change in that co-ordinate is non-zero. For example, if $i = 2$,

$$\frac{\partial |\mathbf{J}|}{\partial x_i^n} = \frac{\partial |\mathbf{J}|}{\partial x_2^n} = \bar{e}_{abc} x_{1,r_a} h_{n,r_b} x_{3,r_c} \quad (29)$$

Finally, to obtain a more compact form, we may rewrite all derivatives with respect to isoparametric co-ordinates in terms of derivatives with respect to global co-ordinates. We find using equation (22) and

$$h_{m,r_a} = x_{j,r_a} h_{m,j}$$

with equations (27) and (28) that

$$\frac{\partial |\mathbf{J}|}{\partial x_i^n} = h_{n,i} |\mathbf{J}|; \quad \frac{\partial u_{k,l}}{\partial x_i^n} = -u_{k,i} h_{n,l} \quad (30)$$

Substituting these into equation (12) yields equation (15).

APPENDIX II: CLOSED FORM EXPRESSIONS FOR THE GRADIENT OF Π
WITH RESPECT TO NODAL CO-ORDINATES FOR TWO-DIMENSIONAL
PLANE STRESS, PLANE STRAIN AND AXISYMMETRIC ELEMENTS

This appendix briefly summarizes the derivations required for the two-dimensional finite elements.

For the plane stress/plane strain element,

$$x_{3,r_3} = t/2 \quad (31)$$

where t is the thickness. Also, either

$$u_3 = 0 \quad (\text{plane strain}) \quad (32)$$

or

$$\tau_{k,3} = 0 \quad (\text{plane stress}) \quad (33)$$

Making these substitutions in equations (15) and (16) gives

$$\frac{\partial \mathcal{Q}^{(m)}}{\partial x_i^n} = \int_{-1}^1 \int_{-1}^1 \left(\frac{1}{2} \tau_{pq} u_{p,q} h_{n,i} - \tau_{kl} u_{k,i} h_{n,l} \right) t |\mathbf{J}| dr_1 dr_2 \quad (34)$$

and

$$\begin{aligned} \frac{\partial \mathcal{W}^{(m)}}{\partial x_i^n} = & \sum_{\text{sides}} \left\{ \int_{-1}^1 (f_k^S u_k)(x_{i,s_1} h_{n,s_1}) (|\mathbf{J}|^S)^{-1} t ds_1 \right\} \\ & + \int_{-1}^1 \int_{-1}^1 f_k^B u_k h_{n,i} t |\mathbf{J}| dr_1 dr_2 \end{aligned} \quad (35)$$

In equations (34) and (35), $|\mathbf{J}|$ is the two-dimensional co-ordinate transformation determinant, $|\mathbf{J}|^S = (x_{p,s_1} x_{p,s_1})^{1/2}$ and s_1 is the isoparametric co-ordinate which varies over the element side.

The derivation for the axisymmetric element is more complicated since the radius enters into the variational indicator. In this derivation, we consider x_2 to be the axis of rotation and consider 1 radian of the structural component. In this case,

$$\mathcal{Q}^{(m)} = \int_{-1}^1 \int_{-1}^1 \frac{1}{2} \tau_{kl} \varepsilon_{kl} |\mathbf{J}| x_1 dr_1 dr_2 \quad (36)$$

where $|\mathbf{J}|$ is the determinant of the Jacobian matrix for the transformation from x_1, x_2 to r_1, r_2 . Taking partial derivatives as before gives

$$\frac{\partial \mathcal{Q}^{(m)}}{\partial x_i^n} = \int_{-1}^1 \int_{-1}^1 \left(x_1 \tau_{kl} |\mathbf{J}| \frac{\partial u_{k,l}}{\partial x_i^n} + \frac{1}{2} \tau_{kl} \varepsilon_{kl} x_1 \frac{\partial |\mathbf{J}|}{\partial x_i^n} + \frac{1}{2} \tau_{kl} \varepsilon_{kl} |\mathbf{J}| \frac{\partial x_1}{\partial x_i^n} \right) dr_1 dr_2 \quad (37)$$

At this point, we note that $u_{3,3}$ is the hoop strain; therefore

$$u_{3,3} = \frac{u_1}{x_1} \quad (38)$$

and

$$du_{3,3} = -\frac{u_{3,3}}{x_1} h_p dx_1^p \quad (39)$$

The other derivatives may be found using the procedure presented in Appendix I. As the final result, we obtain

$$\frac{\partial \mathcal{Q}^{(m)}}{\partial x_i^n} = \int_{-1}^1 \int_{-1}^1 \left[\left(\frac{1}{2} \tau_{pq} u_{p,q} h_{n,i} - \sum_{k,l=1}^2 (\tau_{kl} u_{k,i} h_{n,l}) \right) x_1 + \left(\frac{1}{2} \tau_{pq} u_{p,q} - \tau_{33} u_{3,3} \right) h_n \delta_{i1} \right] |\mathbf{J}| dr_1 dr_2 \quad (40)$$

where $p, q = 1, 2, 3$ but $k, l = 1, 2$ as indicated above, and

$$\frac{\partial W^{(m)}}{\partial x_i^n} = \sum_{\text{sides}} \left\{ \int_{-1}^1 (f_k^S u_k) [x_{i,s_1} h_{n,s_1} (|\mathbf{J}|^S)^{-1} x_1 + h_n \delta_{i1} |\mathbf{J}|^S] ds_1 \right\} + \int_{-1}^1 \int_{-1}^1 f_k^B u_k (h_{n,i} x_1 + h_n \delta_{i1}) |\mathbf{J}| dr_1 dr_2 \quad (41)$$

where $|\mathbf{J}|$, $|\mathbf{J}|^S$ and s_1 are defined as in the two-dimensional plane stress/plane strain case.

We note that all of the results provided in this appendix may also be used in nonlinear elasticity problems provided that the actual strain energy density is substituted for the $\frac{1}{2} \tau_{pq} u_{p,q}$ terms.

REFERENCES

1. K. J. Bathe, *Finite Element Procedures in Engineering Analysis*, Prentice-Hall, Inc., Englewood Cliffs, N.J., 1982.
2. H. Tada, P. C. Paris and G. R. Irwin, *The Stress Analysis of Cracks Handbook*, Del Research Corp., Hellertown, Pa., 1973.
3. D. R. J. Owen and A. J. Fawkes, *Engineering Fracture Mechanics: Numerical Methods and Applications*, Pineridge Press, Swansea, U.K., 1983.
4. T. K. Hellen, 'The finite element calculations of stress intensity factors using energy techniques', 2nd Int. Conf. in Struct. Mech. in Reactor Techn., Paper G5/3, Berlin, Germany (1973).
5. D. M. Parks, 'A stiffness derivative finite element technique for determination of crack tip stress intensity factors', *Int. J. Fract.*, **10**(4), 487-501 (1974).
6. J. R. Rice, 'A path independent integral and the approximate analysis of strain concentration by notches and cracks', *J. Appl. Mech.*, **35**, 379-386 (1968).
7. H. G. deLorenzi, 'On the energy release rate and the J-integral for 3-D crack configurations', *Int. J. Fract.*, **19**, 183-193 (1982).
8. M. Shephard and R. Gallagher (Eds.), *Finite Element Grid Optimization*, A.S.M.E. Monograph, PVP-38, 1979.
9. W. Carpenter and S. Zendegui, 'Optimum nodal locations for a finite element idealization', *Eng. Optim.*, **5**, 215-221 (1982).
10. R. J. Nuismer, 'An energy release rate criterion for mixed mode fracture', *Int. J. Fract.*, **11**(2), 245-250 (1975).
11. D. P. Rooke and D. J. Cartwright, *Compendium of Stress Intensity Factors*, H.M.S.O., London, 1976, pp. 1-120.
12. *ADINA—A Finite Element Program for Automatic Dynamic Incremental Nonlinear Analysis*, ADINA Engineering Report AE 81-1 (1981).
13. K. J. Bathe and T. D. Sussman, 'An algorithm for the construction of optimal finite element meshes in linear elasticity', A.S.M.E., A.M.D., in *Recent Developments in Computing Methods for Nonlinear Solid and Structural Mechanics*, June 1983.
14. R. S. Barsoum, 'On the use of isoparametric finite elements in linear fracture mechanics', *Int. j. numer. methods eng.*, **10**, 25-37 (1976).