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Higher-order sensitivity analysis of finite element method by automatic differentiation

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Abstract To design optimal mechanical structures, design sensitivity analysis technique using higher order derivatives are important. However, usual techniques for computing the derivatives, for example numerical differentiation methods, are hard to apply to real scale structures because of the large amount of computational time and the accumulation of computational errors.

To overcome the problem, we have studied a new approach for higher order sensitivity analysis of the finite element method using automatic differentiation techniques. The method automatically transforms FORTRAN code to special purpose code which computes both the value of the given functional dependence and their derivatives. The algorithm used in the method automatically and efficiently computes accurate values of higher order partial derivatives of a given functional dependence on many variables.

This paper reports the basic principles of the automatic differentiation method and some experiments on the sensitivity analysis of mechanical structures. The original program of structural analysis by the finite element method is implemented in FORTRAN, which is developed by the first author. Using the proposed method, we get more accurate sensitivity and prediction values compared with usual numerical differentiation. We also discuss the effectiveness of the proposed approach for the sensitivity analysis of the mechanical structures.

1 Introduction

The importance of sensitivity analysis using the finite element method (FEM) has been recognized to get higher precision and higher functionalities of mechanical structures in the structural design optimization (Haftka et al. 1986a; Brebbia et al. 1989; Eschenauer et al. 1990). For example, to evaluate dynamical characteristics of structures, modal analysis techniques are used (Ozaki 1988). The optimal mechanical design has been studied by sensitivity analysis using the method. The traditional sensitivity analysis methods are usually direct differentiation method, adjoint variable method, and numerical differentiation method (Adelman et al. 1986; Haftka et al. 1989). Usual techniques for the sensitivity analysis (Haftka et al. 1989; Kleiber and Hisada 1993) require numerically computed partial derivatives of the objective functions (Vanderplaats 1984). Jacobian or Hessian matrices are used to compute optimal values by Newton- or quasi-Newton algorithms (Evtushenko 1985; Ratschek et al. 1988). However, there are several problems for the computation: (1) truncation and rounding errors become large when numerically executing the sensitivity analyses, (2) much computation time is required to compute higher order derivatives to get optimal solutions, and (3) it is difficult to develop programs for the computation of higher order derivatives of a function with very many variables (e.g., Vanhonacker 1980; Belle 1982; Haug et al. 1982; Jawed et al. 1984; Haftka et al. 1986b; Wanxie et al. 1986; Dailey 1989).

To solve the problem, we study a new approach (Ozaki 1991; Ozaki et al. 1992; Ozaki and Kimura 1994) for higher order sensitivity analysis of FEM using automatic differentiation methods. We employ the tool DAFOR, a pre-processor for usual FORTRAN compilers (Berz 1991; Berz 1989; 1990a). Users of the tool first input their FORTRAN code to compute the values of the functional dependence with very many variables for the FEM structural analysis. Next, the tool analyzes the input program and insert statements to compute higher order partial derivatives of the function. Then, the tool automatically generates a special FORTRAN program with sensitivity analysis capability. The method of code generation to compute partial derivatives in many variables is obtained by the automatic differentiation technique whose developers include Iri (1984), Rall (1986), Berz (1989; 1991b), Iri and Kubota (1991), and Griewank et al. (1991). The unique feature of the automatic differentiation method is that the technique can compute higher order partial derivatives with very high accuracy (Ozaki 1991). The generated program is free from both truncation and rounding errors (Iri and Kubota 1991; Griewank et al. 1991). Therefore, by applying the tool, the user can easily carry out sensitivity analysis for optimizing structural design problems.

This paper describes the principles of the automatic differentiation method and reports the computational results of the FEM codes generated by the method applied to a plane truss structure and a machine tool structure. Dixon et al. (1988) theoretically discuss the importance of automatic differentiation techniques for finite element optimization,

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however, they do not show numerical results of the method. On the other hand, in this paper, we emphasize the theory as well as the experimental results. The results indicate that the technique and the use of sensitivity analysis by FEM generated using an automatic differentiation method are very effective in the sense that (1) unlike usual sensitivity analyses for FEM methods (e.g., Fox et al. 1968; Wu and Arora 1986; Haftka et al. 1989; Jao and Arora 1992; Kleiber 1993), the generated program can simultaneously compute the values of partial derivatives of a given function with very high accuracy, and that (2) the values computed by the generated program and the one computed by usual re-analysis by the FEM coincide with each other. The paper is organized as follows: In section 2, the basic principles of the automatic differentiation method is introduced. In section 3, the system configuration for automatic differentiation method is described. In section 4, some experiments to apply the automatic differentiation technique to sensitivity analysis are carried out. In section 5, we give some concluding remarks.

2
Basic principles of automatic differentiation

In this section, we will provide the mathematical background of the theory of the forward mode of the automatic differentiation method. Automatic Differentiation methods are, in general, based on the direct application of the chain rule for computing partial derivatives of a composite function of given function with many variables (Ozaki 1991). In the following, we will describe the outline of the mathematical theory based on Berz (1989; 1990a). We will also provide the mathematical background of the theory of automatic differentiation required for the promised study of non-linearities. It can be viewed as an application of the relatively new field of *Nonarchimedean Analysis*, which allows the introduction of arbitrarily small quantities, infinitesimals, in a rigorous theory of analysis (Berz 1992; 1994).

2.1
Principle of first order partial derivatives using the automatic differentiation

Consider the vector space R^2 of ordered pairs (a_0, a_1), $a_0, a_1 \in R$, in which an addition and a scalar multiplication are defined in the usual way:

$$(a_0, a_1) + (b_0, b_1) = (a_0 + b_0, a_1 + b_1) \tag{1}$$

$$t \cdot (a_0, a_1) = (t \cdot a_0, t \cdot a_1) \tag{2}$$

for $a_0, a_1, b_0, b_1 \in R$. Besides the above addition and scalar multiplication a multiplication between vectors is introduced in the following way:

$$(a_0, a_1) \cdot (b_0, b_1) = (a_0 \cdot b_0, a_0 \cdot b_1 + a_1 \cdot b_0) \tag{3}$$

for $a_0, a_1, b_0, b_1 \in R$. With this definition of a vector multiplication the set of ordered pairs becomes an algebra, denoted by ${}_1D_1$.

Note that the multiplication is the same one would obtain by multiplying $(a_0 + a_1 \cdot x)$ and $(b_0 + b_1 \cdot x)$ and keeping terms linear in x.

Similarly, as in the case of complex numbers, one can identify $(a_0, 0)$ as the real numberes a_0. Although as a complex number, $(0, 1)$ is a root of -1, here it has another interesting property:

$$(0, 1) \cdot (0, 1) = (0, 0), \tag{4}$$

which follows directly from Eq. (3). So $(0, 1)$ is a root of 0. Such a property suggests thinking of $d = (0, 1)$ as something infinitely small; so small in fact that its square vanishes. Consequently, we call $d = (0, 1)$ the differential unit. The first component of the pair (a_0, a_1) is called the real part, and the second component is called the differential part.

It is easy to verify that $(1, 0)$ is a neutral element of multiplication, because according to Eq. (3)

$$(1, 0) \cdot (a_0, a_1) = (a_0, a_1) \cdot (1, 0) = (a_0, a_1) \tag{5}$$

It turns out that (a_0, a_1) has a multiplicative inverse if and only if a_0 is nonzero; so ${}_1D_1$ is not a field. In case $a_0 \neq 0$ the inverse is

$$(a_0, a_1)^{-1} = \left(\frac{1}{a_0} - \frac{a_1}{a_0^2}\right) \tag{6}$$

It is easy to check that in fact $(a_0, a_1)^{-1} \cdot (a_0, a_1) = (1, 0)$. The space ${}_1D_1$ is a subspace of the field R^* introduced in *Nonarchimedean Analysis*. Besides the usual real number, R^* contains a variety of infinitely small and infinitely large quantities. The outstanding result of the theory of Nonstandard Analysis is that differentiation becomes an algebraic problem: a function f is differentiable if and only if for any arbitrary small quantity δ, the real part of the quotient,

$$\frac{f(x + \delta) - f(x)}{\delta}, \tag{7}$$

is independent of the choice of the specific δ. Thus, given any differentiable function f, we can compute its derivatives just by evaluating the formula for a special choice of δ. We choose $\delta = d = (0, 1)$ and thus obtain

$$f'(x) = \Re\left[\frac{f(x + d) - f(x)}{d}\right]$$

or

$$f'(x) = \vartheta[f(x + d) - f(x)] = \vartheta[f(x + d)], \tag{8}$$

where $\Re$ denote the real part, and ϑ denotes the differential part. In the last step use has been made of the fact that $f(x)$ has no differential part. Hence differential algebras are useful to compute derivatives directly, without requiring an analytic formula for the derivatives and without the inaccuracies of numerical techniques.

2.2
Principle of higher order partial derivatives using the Automatic differentiation

We define $N(n, v)$ to be the number of monomials in v variables through order n. We will show that

$$N(n, v) = \frac{(n + v)!}{n!\,v!} = C(n + v, v),$$

where $C(i,j)$ is the familiar bionomial coefficient. First note that the number of monomials with exact order n equals $N(n, v-1)$ because each monomial of exact order n can be written as a monomial with one variable less times the last variable to such a power that the total power equals n. Thus we have $N(n,v) = N(n-1,v) + N(n,v-1)$: the number of monomials in v variables through order n equals the number of relation is satisfied by $C(n+v,v)$. Since also, obviously, $C(1+1,1) = 2 = N(1,1)$, the formula follows by induction.

Now assume that all these N monomials are arranged in a certain manner order by order. For each monomial M, we call I_M the position of M according to the ordering. Conversely, with M_I we denote the I-th monomial of the ordering. Finally, for an I with $M_I = x_1^{i_1}\cdots x_v^{i_v}$, we define $F_I = i_1!\cdots i_v!$.

We now define, in addition, a scalar multiplication and a vector multiplication on R^N in the following way:

$$(a_1,\ldots,a_N) + (b_1,\ldots,b_N) = (a_1+b_1,\ldots,a_N+b_N) \tag{9}$$

$$t\cdot(a_1,\ldots,a_N) = (t\cdot a_1,\ldots,t\cdot a_N) \tag{10}$$

$$(a_1,\ldots,a_N)\cdot(b_1,\ldots,b_N) = (c_1,\ldots,c_N) \tag{11}$$

where the coefficients c_i are defined as follows:

$$c_i = F_i \sum_{\substack{0\le v,\mu\le N\\ Mv\cdot M\mu = M_i}} \frac{a_v\cdot b_\mu}{F_v\cdot F_\mu} \tag{12}$$

To help clarify these definitions, let us look at the case of two variables and second order. In this case, we have $n=2$ and $v=2$. There $N = C(2+2,2) = 6$ monomials in two variables, namely,

$$1, x, y, xx, xy, yy. \tag{13}$$

As an example, using the ordering in Eq. (13), we have $I_{xy} = 5$ and $M_3 = y$. Using the ordering in Eq. (13), we obtain for c_1 through c_6 in Eq. (12):

$$\begin{aligned}
c_1 &= a_1\cdot b_1\\
c_2 &= a_1\cdot b_2 + a_2\cdot b_1\\
c_3 &= a_1\cdot b_3 + a_3\cdot b_1\\
c_4 &= 2\cdot(a_1\cdot b_4/2 + a_2\cdot b_2 + a_4\cdot b_1/2)\\
c_5 &= a_1\cdot b_5 + a_2\cdot b_3 + a_3\cdot b_2 + a_5\cdot b_1\\
c_6 &= 2\cdot(a_1\cdot b_6/2 + a_3\cdot b_3 + a_6\cdot b_1/2).
\end{aligned} \tag{14}$$

On ${}_nD_v$ we introduce a third operation ∂_i:

$$\partial_i(a_1,\cdots,a_N) = (c_1,\cdots,c_N) \tag{15}$$

with

$$c_i = \begin{cases} 0 & \text{if } M_i \text{ has order } n \\ a_{I(M_i\cdot x_v)} & \text{otherwise} \end{cases} \tag{16}$$

So ∂_v moves the derivatives around in the vector. Suppose a vector contains the derivatives of the function f; then applying ∂_v to in one obtains the derivatives of $\partial f/\partial x_v$ through one order less.

Although in ${}_1D_1$, $d = (0,1)$ was an infinitely small quantity, here we have a whole variety of infinitely small quantities with the property that high-enough powers of them vanish. We give special names to the ones in components I belonging to first-order monomials, denoting them by dM_I. In the example of ${}_2D_2$, we have $dx = (0,1,0,0,0,0)$, and $dy = (0,0,1,0,0,0,0)$. It then follows from the theory of *Nonarchimedean Analysis* that instead of Eq. (8) we obtain

$$f(x+dx, y+dy) = \left(f, \frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial^2 f}{\partial x^2}, \frac{\partial^2 f}{\partial x \partial y}, \frac{\partial^2 f}{\partial y^2}\right)(x,y). \tag{17}$$

In the general case of v variables and order n, after evaluating f in the differential algebra one obtains

$$\frac{\partial^{i_1+i_2+\cdots+i_v} f}{\partial x_1^{i_1}\partial x_2^{i_2}\cdots\partial x_v^{i_v}} = c_{I(x_1^{i_1}\cdots x_v^{i_v})} \tag{18}$$

where $I(x_1^{i_1}\cdots x_v^{i_v})$ is the index of the monomial $(x_1^{i_1}\cdots x_v^{i_v})$, as defined in the beginning of this section.

3 System configuration for the automatic differentiation method

Figure 1 shows the system configuration and usage of DAFOR (Berz 1989; 1991; Ozaki 1991). The system consists of two components: the first component is a pre-complier for generating a FORTRAN source code for the computation by automatic differentiation; and the second component is a library for computing fundamental functions (e.g., sin x, e^x) used for the automatic differentiation method. Figure 2 shows sample code fragments of an input FORTRAN program for FEM analysis. Figure 3 shows the resulting code fragment generated by DAFOR. The program contains special purpose subroutine call statements to compute higher order partial derivatives of a given function (e.g., CALL DACOP, CALL DASUB in the figure).

4 Sensitivity analysis on mechanical structures using an automatic differentiation technique

We have applied the automatic differentiation method to sensitivity analysis problems with the FEM, which is the most popular in structural analyses. In the case studies described below, the automatic differentiation method is used to investigate the sensitivity of design variables of mechanical structures. The automatic differentiation method can be applied to both linear and non-linear equations (Berz 1989; Ozaki 1991), if the equations are n times differentiable. Moreover, using the method, we can highly accurately compute higher order partial derivatives in many variables. In the case studies, we have applied the method to two-dimensional linear FEM problems of structural analyses (Ozaki 1989).

4.1 Example1: First- and higher-order sensitivity analysis

The code of sensitivity analysis of FEM using automatic differentiation has been applied to a plane truss structure. The model is a simple static model shown in Fig. 4, by which we will simulate a train passing over an iron bridge. This consists of eight nodes and thirteen truss elements. The

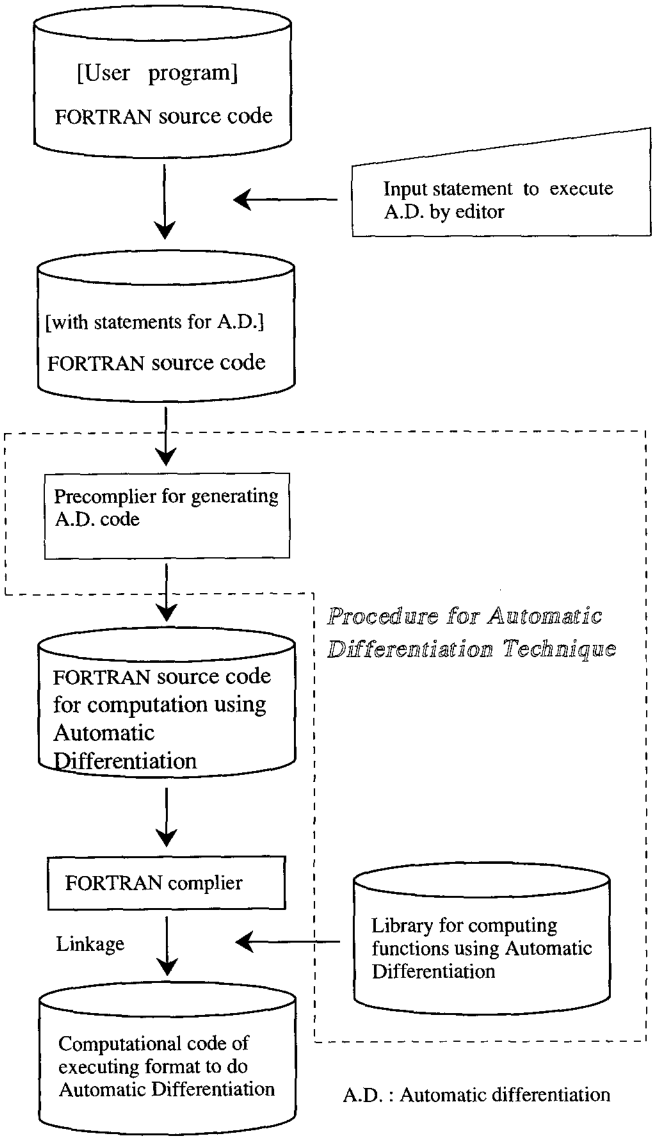

Fig. 1. System configuration of automatic differentiation technique

```
*PRE-NO-NV NO=3,NV=6                    -------              inserted statement
C  Program plane truss for sensitivity analysis  using AutomaticDifferentiation

      IMPLICIT DOUBLE PRECISION(A-H,O-Z)
      DIMENSION XX(10),YY(10),II(15),JJ(15),EE(15),AA(15),DX(50),
     &          DY(50),TK(20),TFD(20),TU(20),EK(4,4),W(4)
      OPEN(5,FILE='DATA')
      READ(5,*) NP,NE,NB,NF
      DO 100 I=1,NP
         READ(5,*) I,XX(I),YY(I)
 100  CONTINUE
            .
            .
      DO 300 I=1,NF
         READ(5,*) I,TFD(2*I-1),TFD(2*I)
 300  CONTINUE
      DO 310 I=1,NF
*PRE-INPUT I TF(2*I-1)=TFD(2*I-1) 'X-FORCE            -- inserted statement
 310  CONTINUE
      DO 320 I=1,NF
*PRE-INPUT I TF(2*I)=TFD(2*I) 'Y-FORCE'  --           inserted statement
 320  CONTINUE
            .
            .
*PRE-OUTPUT(6) TU(I) 'RESULT OF DISPLACEMENT'
            .                                   -- inserted statement
            .
      END
```

Fig. 2. Fortran program for higher-order sensitivity analysis using an automatic differentiation technique

boundary conditions are that the node 7 and 8 are fixed, and that the nodes 1, 2, and 3 respectively have the loads 10,000 kgf, 20,000 kgf, and 10,000 kgf. Using the model, we have carried out the following two experiments.

The two experiments are to compute the values of first and higher order partial derivatives and to predict the deflection of each node and the stress of each element against radius of each element. The object to compute the values of higher order partial derivatives is to indicate the effectiveness of Taylor series expansion using derivatives of higher order when the machine structures are changing greatly during optimization. In particular, the method is very effective when the connection of object function and design variables is non-linear. The relation of the deflection of each node against the radius of each element and the stress of each element against the radius of each element is non-linear. The sensitivity analysis with respect to the deflection of each node against the radius of each element is executed. We show an analytical model of each element in Fig. 4. The sensitivity with respect to deflection of each node against the radius of the element 1 through 13 is computed. The highest sensitivity of node 2 against the radius of each element is given in the case of radius of element 2. The values of first and higher order partial derivatives with respect to the displacement of node 2 against the radius of element 2 is shown in Table 1. Regarding the sensitivity analysis of the values of responses according to the value of changing design variables, the first and higher order partial derivatives were computed in Table 1. The objective of this analysis is to examine the effectiveness of higher order Taylor expansions in the presence of non-linearity. When we changed the values of radius of the element 2 by 1%, 5%, 10%, 20%, 30%, 40%, and 50% increases, we obtained the results shown in Table 2 by computing the displacement of node 2 by the first and higher order partial derivatives obtained using automatic differentiation. The result of direct re-computation by FEM above the condition is shown in Table 2. The results of the displacement of node 2 predicted by the first order sensitivity analysis using an automatic differentiation and the ones by the direct re-computation by FEM do not coincide with each other when the changes of design variables are large, on the other hand the results of the displacement of node 2 predicted by the higher order sensitivity analysis using automatic differentiation and the ones by the direct re-computation by FEM coincide with each other even if the changes are large. Figure 5 illustrates the results of the computation shown in Table 2, and Fig. 6 illustrates the values of differences between the results predicted by first and higher order sensitivity analysis and re-computational values of the displacement of node 2 by FEM.

```
*PRE-NO-NV NO=    3 ,NV=6
*        MAIN PROGRAM OFDA
         IMPLICIT DOUBLE PRECISION(A-H,O-Z)
         INTEGER NODA,NVDA
         COMMON /DANONV/NODA,NVDA
         NODA = 1
         NVDA =  6
         CALL DAINI(NODA,NVDA,1)
         CALL DAINIT
         CALL MAIN
         STOP
         END
         SUBROUTINE DAINIT
         IMPLICIT DOUBLE PRECISION(A-H,O-Z)
         INTEGER NODA,NVDA
         COMMON /DANONV/NODA,NVDA
         RETURN
         END


*DA      B(I)=B(I)-A(I,K)*B(K)                              *FOX
         CALL DACOP(B  (I ),ISCRDA(1+IDAA))
         RSCRRI(2+IDAA) = A    (I  ,K    )
         CALL DACOP(B   (K   ),ISCRDA( 3+IDAA)
         CALL DACMU(ISCRDA(3+IDAA),1.D0*RSCRRI(2+IDAA),
        *ISCRDA(4+IDAA))
         CALL DASUB(ISCRDA(1+IDAA),ISCRDA(4+IDAA),
        *ISCRDA(5+IDAA))
          CALL DACOP(ISCRDA(5+IDAA),B  (I ))
*         B(I)=B(I)-A(I,K)*B(K)        ----- This statement is converted to the
                                       above nine statements for automatic differentiation.
```

Fig. 3. FEM code fragment generated by automatic differentiation technique

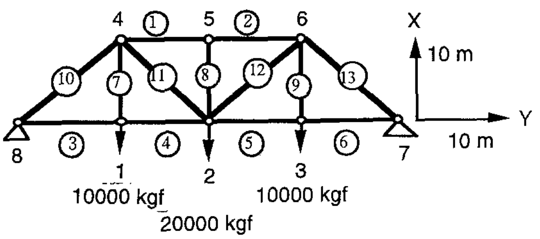

Fig. 4. Analytical model for higher order sensitivity analysis

Table 1. Displacement sensitivity of node 2 against radius of element 2

	Displacement sensitivity of node 2 against radius of element 2
Value of first order derivatives	$9.0946*10^{-3}$
Value of second order derivatives	$-2.7284*10^{-3}$
Value of third order derivatives	$1.0914*10^{-3}$

Table 2. Displacement expected from sensitivity analysis using automatic differentiation increasing radius of element 2

unit (mm)

		Displacement expected from sensitivity analysis using automatic differentiation Original radius of element 2: 100 mm						
		1% increase	5% increase	10% increase	20% increase	30% increase	40% increase	50% increase
A.D.	First order	2.18653 (0.01%)	2.15015 (0.15%)	2.10468 (0.57%)	2.01373 (2.09%)	1.92279 (4.34%)	1.83184 (7.15%)	1.74090 (10.40%)
	Second order	2.18667 (0.0%)	2.15356 (0.0%)	2.11832 (0.07%)	2.06830 (0.57%)	2.04556 (1.77%)	2.05011 (3.91%)	2.08194 (7.15%)
	Third order	2.18667 (0.0%)	2.15333 (0.0%)	2.11650 (0.01%)	2.05375 (0.14%)	1.99645 (0.67%)	1.93370 (1.99%)	1.85458 (4.55%)
Re-analysis by FEM		2.18667	2.15335	2.11670	2.05668	2.00997	1.97290	1.94300

(%): difference value between expected value and re-analysis by FEM
A.D.: Automatic Differentiation

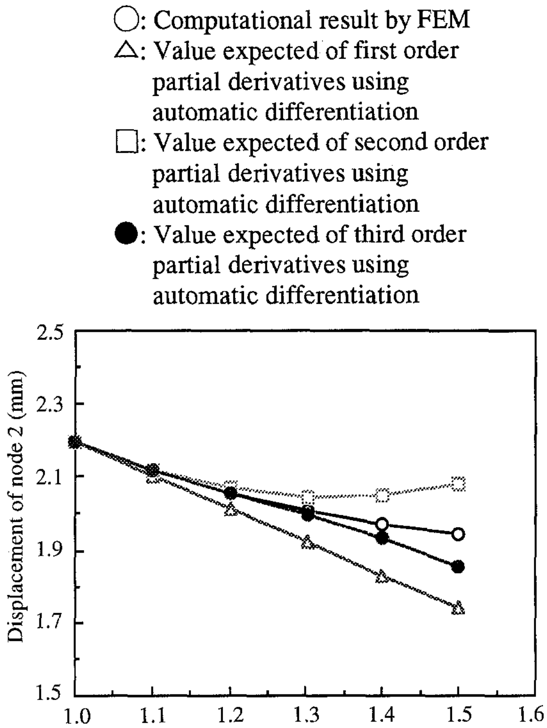

Fig. 5. Value expected from high order partial derivatives using automatic differentiation and computational value by FEM

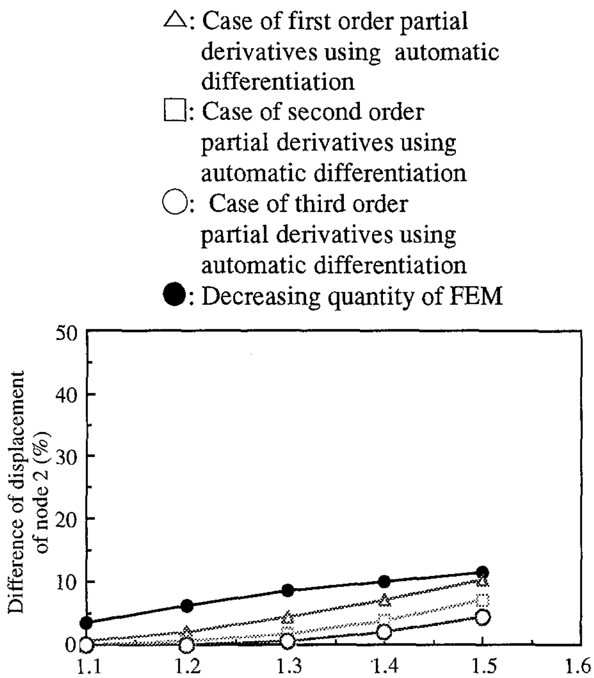

Fig. 6. Difference between high order partial derivatives using automatic differentiation and computational value by FEM

The second experiment is the sensitivity analysis of the stress important for fracture mechanics. The sensitivity analysis of the stress of each element with respect to the radius of each element is executed. The sensitivity of the stress of each element with respect to the radius of the element 1 through 13 is computed. The highest sensitivity of element against radius of each element is the case of the radius of element 2. The values of first and higher order partial derivatives of the stress of element 2 with respect to radius of the element 2 is shown in Table 3. Regarding the sensitivity analysis of the values of responses according to the value of changing design variables, the first and higher order partial derivatives were computed using automatic differentiation in Table 3. The objective of this analysis is to examine the effectiveness of higher order derivatives to describe non-linearity. When we changed the values of radius of the element 2 to 1%, 5%, 10%, 20%, 30%, 40% and 50% increases, we obtained the results shown in Table 4 by computing the compressive stress of element 2 by higher order partial derivatives obtained using automatic differentiation. The result of direct re-computation by FEM above the condition is shown in Table 4. The results of the compressive stress of element 2 predicted by the first order sensitivity analysis using automatic differentiation and the ones by the direct re-computation by FEM do not coincide with each other when the changes of design variables are large; on the other hand the results of the compressive stress of element 2 predicted by the higher order sensitivity analysis and the ones by the direct re-computation by FEM coincide with each other even if the changes are large. Figure 7 illustrates the results of the computation shown in Table 4, and Fig. 8 illustrates the values of differences between the results predicted by first and higher order sensitivity analysis and re-computed values of the compressive stress of element 2 by FEM.

Table 3. Compressive stress sensitivity of element 2 against radius of element 2

	Stress sensitivity of element 2 against radius of element 2 (kgf/mm^3)
Value of first order derivatives	$1.9099*10^{-2}$
Value of second order derivatives	$-5.7296*10^{-3}$
Value of third order derivatives	$2.2918*10^{-3}$

4.2 Example 2: Sensitivity analysis of a machine tool structure

The next example is the analysis of a two dimensional plane strain problem of a machine tool structure, which is a typical example of large scale structural analysis problems (Ozaki 1988). The structural model is shown in Fig. 9, by which we will simulate a two dimensional model of a machine tool. This consists of twenty eight nodes and thirty two elements. The boundary conditions are that the nodes 13, 26, 11 and 23 respectively have the loads 10 kgf, 10 kgf, 5 kgf, and 5 kgf, and that the nodes 20, 21, 22, 25, and 28 are fixed.

In the first experiment, we want to execute an experiment for the purpose of sensitivity analysis of the important principal stress from the viewpoint of fracture mechanics for the mechanical structure. The objective of the sensitivity analysis is to search for the highest principal stress among the thirty two element numbers against the loads of each node. The

Table 4. Compressive stress expected from sensitivity analysis using automatic differentiation increasing radius of element 2

		Compressive stress expected from sensitivity analysis using automatic differentiation Original radius of element 2 : 100 mm					unit (kgf/m^2)	
		1% increase	5% increase	10% increase	20% increase	30% increase	40% increase	50% increase
A.D.	First order	−0.9358 (0.03%)	−0.8594 (0.8%)	−0.7639 (3.2%)	−0.5730 (13.6%)	−0.3820 (32.4%)	−0.1910 (60.8%)	−0.0000 (100%)
	Second order	−0.9361 (0.00%)	−0.8666 (0.05%)	−0.7926 (0.4%)	−0.6875 (3.7%)	−0.6398 (13.2%)	−0.6493 (33.3%)	−0.7162 (68.8%)
	Third order	−0.9361 (0.00%)	−0.8661 (0.00%)	−0.7888 (0.05%)	−0.6570 (0.9%)	−0.5367 (5.0%)	−0.4049 (16.9%)	−0.2387 (43.8%)
Re-analysis by FEM		−0.9361	−0.8661	−0.7892	−0.6632	−0.5651	−0.4872	−0.4244

(%): difference value between expected value and Re-analysis by FEM
A.D.: Automatic Differentiation

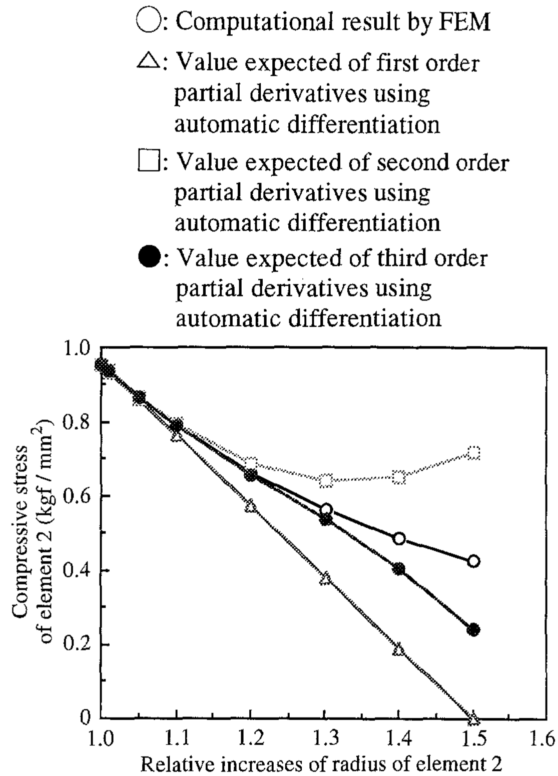

Fig. 7. Value expected from high order partial derivatives using automatic differentiation and computational value by FEM

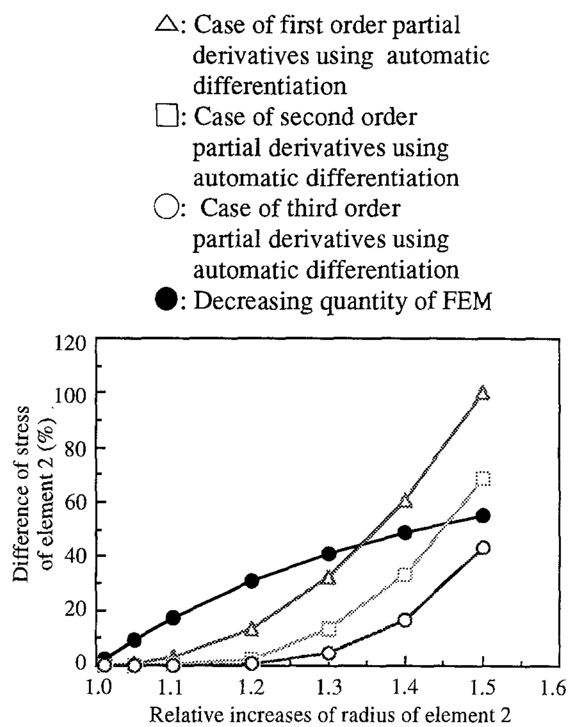

Fig. 8. Difference between high order partial derivatives using automatic differentiation and computational value by FEM

design parameters for the above objective are the loads of the nodes 11, 13, 23, and 26. The sensitivity analysis of the principal stress of the all elements were executed as to the design parameters using an automatic differentiation method. The

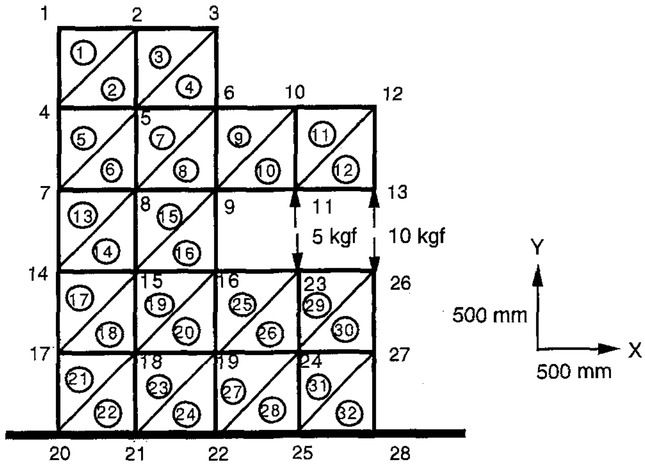

Fig. 9. Analytical model for machine tool structures

first order partial derivatives shown in Table 5 were computed for sensitivity analysis by FEM using an automatic differentiation method. The objects of the sensitivity analysis shown in Table 5 are the elements of the higher principal stress in the all elements, that is elements 10, 12, 15, 16, and 25.

In the next step, we executed an experiment to predict the principal stress values of the elements by making use of the first order partial derivatives obtained using automatic differentiation when the values of the design parameters change. In the experiment, because node 13 gives the highest effect to the principal stress of the element 10, 12, 15, and 16, we hanged the values of load of node 13 (10 Kgf) to 0.1%, 0.5%, 1%, 5%, and 10% increases. The predicted values of the principal stress of each element are shown in Table 6. The result of the sensitivity analysis by automatic differentiation and the direct re-computation by FEM perfectly coincide with each other. In the second experiment, we studied sensitivity analysis based on automatic differentiation in comparison with other methods of sensitivity analysis. The traditional method of sensitivity analysis is based on the design of mechanical structures, for example the method of direct differentiation method, adjoint variable method, and numerical differentiation method (Adelman 1986; Haftka 1989). The numerical differentiation method is very popular and easy in the above sensitivity analysis method, and the numerical differentiation method can also be applied to compute partial derivatives concerning linear equation and non-linear equations. In this experiment, we would like to execute an experiment to study their computational accuracy compared to that of the automatic differentiation method. The quantity evaluated in this experiment is the important principal stress from a viewpoint of fracture mechanics for the mechanical structure. Sensitivity analysis is performed to determine the principal stress of the each elements against the loads of vertical direction. The first order partial derivative computed the

Table 5. Sensitivity of principal stress against each load

Element number (Principal stress)	Sensitivity of principal stress against load (Value of first order partial derivatives)			
	Node 13 10 Kg	Node 11 5 Kg	Node 23 −10 Kg	Node 26 −5 Kg
10 $6.37902*10^{-2}$	$5.10150*10^{-3}$	$2.55557*10^{-3}$	$-1.58716*10^{-7}$	$3.47793*10^{-7}$
12 $2.24642*10^{-2}$	$2.33569*10^{-3}$	$-1.78527*10^{-4}$	$-3.49382*10^{-9}$	$7.65595*10^{-9}$
15 $3.13667*10^{-2}$	$2.37553*10^{-3}$	$1.50970*10^{-3}$	$8.57690*10^{-6}$	$-1.05802*10^{-5}$
16 $3.28440*10^{-2}$	$2.32745*10^{-3}$	$1.57481*10^{-3}$	$-4.07929*10^{-5}$	$-1.49148*10^{-4}$
25 $6.00691*10^{-3}$	$3.80131*10^{-4}$	$2.61129*10^{-4}$	$7.63843*10^{-4}$	$-4.71917*10^{-4}$

Table 6. The Principal Stress expected from sensitivity analysis using automatic differentiation increasing load of node 13

Element number		Principal Stress using automatic differentiation Original load of node 13 : 10 kgf			unit (kgf/mm^2)	
		0.1% increase 0.01 kgf	0.5% increase 0.05 kgf	1.0% increase 0.1 kgf	5% increase 0.5 kgf	10% increase 1.0 kgf
10	A.D.	$6.3841*10^{-2}$	$6.4045*10^{-2}$	$6.4300*10^{-2}$	$6.6341*10^{-2}$	$6.889*10^{-2}$
$6.3790*10^{-2}$	Re-analysis by FEM	$6.3841*10^{-2}$	$6.4045*10^{-2}$	$6.4300*10^{-2}$	$6.6341*10^{-2}$	$6.889*10^{-2}$
16	A.D.	$3.2867*10^{-2}$	$3.2960*10^{-2}$	$3.3077*10^{-2}$	$3.4008*10^{-2}$	$3.5171*10^{-2}$
$3.2844*10^{-2}$	Re-analysis by FEM	$3.2867*10^{-2}$	$3.2960*10^{-2}$	$3.3077*10^{-2}$	$3.4008*10^{-2}$	$3.5171*10^{-2}$
15	A. D.	$3.1390*10^{-2}$	$3.1485*10^{-2}$	$3.1604*10^{-2}$	$3.2554*10^{-2}$	$3.3742*10^{-2}$
$3.1367*10^{-2}$	Re-analysis by FEM	$3.1390*10^{-2}$	$3.1485*10^{-2}$	$3.1604*10^{-2}$	$3.2554*10^{-2}$	$3.3742*10^{-2}$
12	A.D.	$2.2488*10^{-2}$	$2.2581*10^{-2}$	$2.2698*10^{-2}$	$2.3632*10^{-2}$	$2.4800*10^{-2}$
$2.2464*10^{-2}$	Re-analysis by FEM	$2.2488*10^{-2}$	$2.2581*10^{-2}$	$2.2698*10^{-2}$	$2.3632*10^{-2}$	$2.4800*10^{-2}$

A.D.: Automatic Differentiation

Table 7. Comparison of computational accuracy with automatic differentiation and numerical differentiation

Element number of object (Principal stress: Kgf/mm²)		Sensitivity of the principal stress against load of node 13 (maximum load) load of node 13 : 10 Kgf				
		0.1% [1] (0.01 Kgf)	0.5% (0.05 Kgf)	1.0% (0.10 Kgf)	5% (0.50 Kgf)	10% (1.00 Kgf)
10	A.D.			$5.1015*10^{-3}$		
$(6.3790*10^{-2})$ [2]	N.D.	$5.1020*10^{-3}$	$5.1000*10^{-3}$	$5.1018*10^{-3}$	$5.1025*10^{-3}$	$5.1035*10^{-3}$
16	A.D.			$2.3274*10^{-3}$		
$(3.2844*10^{-2})$	N.D.	$2.3279*10^{-3}$	$2.3274*10^{-3}$	$2.3275*10^{-3}$	$2.3274*10^{-3}$	$2.3274*10^{-3}$
15	A.D.			$2.3755*10^{-3}$		
$(3.1367*10^{-2})$	N.D.	$2.3750*10^{-3}$	$2.3754*10^{-3}$	$2.3755*10^{-3}$	$2.3756*10^{-3}$	$2.3757*10^{-3}$
12	A.D.			$2.3357*10^{-3}$		
$(2.2464*10^{-2})$	N.D.	$2.3350*10^{-3}$	$2.3356*10^{-3}$	$2.3357*10^{-3}$	$2.3357*10^{-3}$	$2.3357*10^{-3}$

A.D.: Automatic Differentiation
N.D.: Numerical Differentiation
[1] differential width
[2] Principal stress value of each element

sensitivity analysis by FEM using an automatic differentiation method were indicated in Table 6 by the previous experiment. As a consequence, the vertical load of node 13 experienced the highest effect to the principal stress of the elements 10, 12, 15, and 16, and we apply the above results in this experiment. The result of the sensitivity analysis by the automatic differentiation method and the numerical differentiation method are shown in Table 7. We select the differential width of 0.1%, 0.5% 1%, 5%, and 10% for the values of load of the node 13 (10 kgf) in the sensitivity analysis based on numerical differentiation, because for these values, the result computed using an automatic differentiation method and the direct re-computation by FEM perfectly coincide with each other. The result of sensitivity analysis using numerical differentiation are different; the values of first partial derivatives are shown in Table 7 as a function of the differential width, and the numerical differentiation method must change the differential width. The computational error is increased by rounding error and truncation error in the numerical computational process of sensitivity analysis, and therefore the numerical differentiation method is not useful from the viewpoint of computational accuracy and computational effort. The automatic differentiation method is very effective from the viewpoint of computational accuracy and computational labor in comparison with numerical differentiation method.

In the third experiment, we have investigated computation costs of the sensitivity analysis by FEM using the automatic differentiation method. The structural analysts would like to want the sensitivity analysis of the plural objective functions against the design variables when the optimum design is executed the design for the mechanical structures. We have computered the sensitivity analysis of the plural objective functions by the sensitivity analysis code of FEM for the plane strain analysis using the automatic differentiation method. The design parameters are the loads of nodes (four loads) and the Young's modulus of the all elements (thirty two elements), and the evaluation items are each the stress, shearing stress, and two kinds of the principal stresses of the X direction and the Y direction. We have executed the sensitivity analysis when increasing the number of objective functions. Figure 10 shows the computation of the sensitivity analysis when the

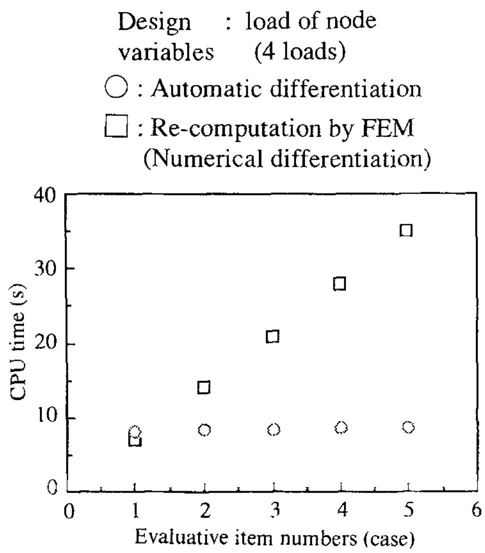

Fig. 10. Computational time increasing evaluation item

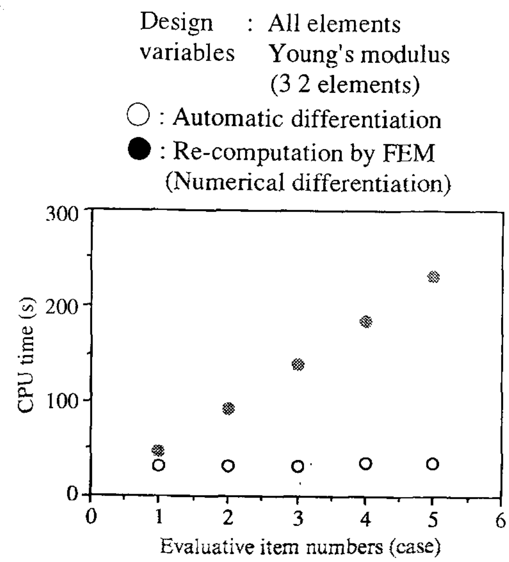

Fig. 11. Computational time increasing evaluation item

Table 8. Sensitivity of node against Young's modulus of element

Node number	Sensitivity of node against Young's modulus of element				
13	$-1.71634*10^{-7}$	$-1.47323*10^{-7}$	$-1.40783*10^{-8}$	$-7.75710*10^{-8}$	$-6.08862*10^{-8}$
	EN 9	EN 16	EN 8	EN 10	EN 6
12	$-1.71768*10^{-7}$	$-1.47321*10^{-7}$	$-1.40801*10^{-7}$	$-7.70304*10^{-8}$	$-6.08888*10^{-8}$
	EN 9	EN 16	EN 8	EN 10	EN 6
11	$-1.06680*10^{-7}$	$-9.96540*10^{-8}$	$-6.97619*10^{-8}$	$-5.19272*10^{-8}$	$-3.35183*10^{-8}$
	EN 16	EN 9	EN 8	EN 10	EN 6
10	$-1.06631*10^{-7}$	$-1.02653*10^{-7}$	$-7.01887*10^{-8}$	$-3.92238*10^{-8}$	$-3.35796*10^{-8}$
	EN 16	EN 9	EN 8	EN 10	EN 6

EN: element number

design parameters are the loads of the nodes(four loads). Figure 11 shows the computation of the sensitivity analysis when the design parameters are the Young's modulus of the all elements (thirty two elements). The increases of the computational time are very little against the increases of evaluative items from the Fig. 10 and 11. On the other hand, the evaluation items against the design parameters are increasing, the usual sensitivity analysis using the numerical differential method rapidly increases the computational time. Therefore, the sensitivity analysis for FEM using the automatic differentiation method is the very effective when the plural evaluation items must be computered. This suggests the superiority of our automatic differentiation method.

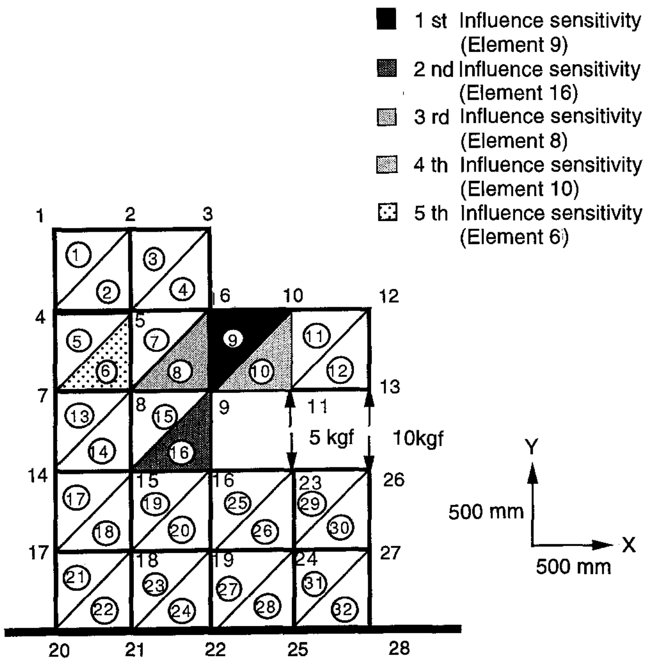

Fig. 12. Distribution chart of the computational sensitivity

4.3
Example 3: Optimum design of a machine tool structure by sensitivity analysis

We tried to find the optimum design of a machine tool structure by sensitivity analysis using an automatic differentiation technique. In this experiment, we use the machine tool structure shown in Fig. 9 of the previous section. The machine tool structure has problems in the form of deflection of the point of contact of the grinding wheel and the cut product, because

Table 9. The computational result using FEM when Young's modulus increase 5 times

Node number	Computational result when Young's modulus increase 5 times unit (um)		
	Element 6	Element 16	Element 9
13	19.2884	18.2772	17.6185
21.0994 um	8.5%	13.4%	16.5%
12	18.6262	17.6097	16.9525
20.4373 um	8.8%	13.7%	16.7%
11	10.6845	9.6286	9.5276
11.6789 um	8.5%	17.9%	18.8%
10	10.2900	9.2369	9.0452
11.2861 um	8.8%	18.6%	20.4%

per cents(%): decreasing ratio

Table 10. The deflection of processing point when the Young's modulus of the element 9 increases in order to optimize design

Node number	Computational result by FEM when the Young's modulus of the element 9 increases unit (um)			
E = 21000	10%	2 times	5 times	10 times
Kgf/mm^2	23100	42000	105000	210000
13	20.7674	19.1224	17.6185	17.0036
21.0994 um	1.9%	9.5%	16.5%	19.4%
12	20.1051	18.4585	16.9525	16.3367
20.4373 um	1.5%	9.3%	16.7%	20.1%
11	11.4851	10.4916	9.5276	9.1180
11.6789 um	1.7%	10.3%	18.8%	22.2%
10	11.0863	10.0555	9.0452	8.6132
11.2861 um	1.8%	10.6%	20.4%	23.9%

per cents(%): decreasing quantity

Table 11. Computational result of displacement of each node when Young's modulus of effective elements increase

Node Number	Computational result of displacement of each node by FEM when Young's modulus of effective elements increase											unit (um)
	2 times increase of Young's modulus, E = 42000 Kgf/mm²				5 times increase Young's modulus, E = 105000 Kgf/mm²				10 times increase of Young's E = 210000 Kgf/mm²			
	elements increase Young's modulus				elements increase Young's modulus				elements increase Young's modulus			
	9	9,16	8,9,16	6,8,9,10,16	9	9,16	8,9,16	6,8,9,10,.16	9	9,16	8,9,16	6,8,9,10,16
13	19.1224	17.4321	15.6687	14.3966	17.6185	14.7012	11.5078	9.8135	17.0036	13.6080	9.8487	8.1405
21.0994 um	9.5%	17.5%	25.6%	31.8%	16.5%	30.0%	45.5%	53.6%	19.4%	35.5%	53.6%	61.6%
12	18.4585	16.7682	15.0046	13.7400	16.9525	14.0353	10.8417	9.1625	16.3367	12.9412	9.1817	7.4920
20.4373 um	9.3%	17.6%	26.5%	32.8%	16.7%	31.4%	47.1%	54.9%	20.1%	39.7%	54.9%	63.2%
11	10.4916	9.2691	8.3899	7.6297	9.5276	7.4219	5.8350	4.8641	9.1180	6.6701	4.8095	3.8551
11.6789 um	10.3%	20.5%	28.2%	35.0%	18.8%	36.8%	50.4%	58.1%	22.2%	42.7%	59.0%	66.7%
10	10.0556	8.8337	7.9500	7.3670	9.0452	6.9403	5.3483	4.7323	8.6132	6.1659	4.3017	3.7832
11.2861 um	10.6%	22.1%	30.1%	34.5%	20.4%	38.9%	53.1%	58.4%	23.9%	45.1%	61.9%	66.4%

per cents(%): decreasing ratio

grinding accuracy is dependent on the deformation of the grinding wheel (Ozaki 1988; 1991), therefore we want that deformation of the grinding wheel reduced as much as possible to realize a high quality product. We hope that the stiffness of the parts affecting deflection of the grinding wheel are strong. To obtain a high quality product, the objective of the sensitivity analysis is to explore the optimal Young's modulus of the most effective elements in order to minimize the deflections of the nodes 12 and 13, which shows the largest values among the nodes. To get the sensitivities of the deflection of each node, we determine the values of Young's modulus of all the elements as design parameters. The objectives of the experiment are (1) to get the sensitivity of the deflections of the nodes, and (2) to optimize stiffness of the machine tool structure in order to minimize the deflections of the nodes connected grinding accuracy.

In the first step, we computed the sensitivity of the node delection values against the changes of Young's modulus. The results of the analysis are shown in Table 8, which describes the effects to the nodes 12, 13, 11, and 10. For example, on the node 13, the deflection value is the largest, and the elements 9, 16, 8, 10, and 6 give the effects of increasing order. Figure 12 shows the distribution chart for sensitivity describing the effects to the Young's modulus of each element against the node 13. To validate the results of sensitivity analysis by the automatic differentiation method, we have carried out direct FEM analyses, in which we have changed the Young's modulus of the elements 9, 16, and 6 from the original to a value increased by a factor of five. We compared the deflection values of the elements 9, 16, and 6. The results are shown in Table 9, in which we find that the deflection values decrease according to the increases of the effects of deflections of the nodes.

In the second step, it is desired to reduce the deflection of the point connected to the grinding wheel as much as possible in order to realize a high quality product. It is assumed that the grinding wheel is fitted on node 11 and node 13 in the machine tool structure shown in Fig. 9. We assume that the objective function for optimization is the deflection of node 13. The previous sensitivity analysis showed that the Young's modulus of elements 9 is the optimal Young's modulus of the most effective elements in order to minimize the deflection of the node 13. The computational result is shown in Table 10 when we increase the Young's modulus of the elements 9 in order to minimize the deflection value of nodes 13, 12, 11, and 10.

In the third step, we executed an experiment in order to minimize the deflection of the nodes fitted the grinding wheel when the Young's modulus of the multi elements increases at the same time. In the experiment, because the element 9, 16, 8, 10, and 6 give a higher effect to the deflections of the nodes 13, 12, 11, and 10, we changed the values of Young's modulus of the each element to 2 times, 5 times, and 10 times its original value. The computational result of deflection of each node by FEM are shown in Table 11, when the Young's modulus of the effective multi elements increases at the same time. In the modified design of the above experiment, we have obtained optimum design that the deflection of the nodes 13 and 12 are minimized compared to the Young's modulus of the elements 9 and 16 to 5 times increases with the Young's modulus of the elements 9 to 10 times increases. The mechanical structure as to machine tool structure required higher quality and higher precision are given damage to lose the equilibrium connection around the objective parts optimized, when the changing design are large. We have gotten that the optimal design is very effectiveness and practical use by a few changing design in this experiment.

5 Concluding remarks

Using automatic differentiation techniques, we observed the following advantages in the analyses.

(1) We can very easily and quickly execute sensitivity analysis of structural design problems.
(2) We can very easily execute optimal design on machine tool structure by sensitivity analysis.
(3) We can also predict the effects of changing design parameters with high accuracy.
The most remarkable feature of the automatic differentiation method is that the method can simultaneously compute the values of higher order partial derivatives. This results in the following effects in the sensitivity analyses.
(4) Our method becomes superior to the conventional ones using numerical differentiation, because it is not sensitive to the rounding and truncation errors associated with the numerical computational process of sensitivity analysis.
(5) Our method is very effective when there are non-linear dependences in on the design parameters.

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