"ON THE ERROR ESTIMATION IN THE FINITE-DIFFERENCE ENERGY METHOD IN CONTINUUM MECHANICS".

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ABSTRACT : The system of numerically algebraic equations resulting from FDE method for a class of Variational problems of the fourth order is represented by a differential equation with infinite terms. By using the perturbation method for the solution of this differential equation, it has been found that the first order solution is an estimate of error in FDE method. This estimate has been determined for the comparative study of three difference approximations and is illustrated by a model example.

1. THE FINITE-DIFFERENCE ENERGY METHOD.

The difficulties associated with conventional finite difference analysis [Ref. (1)] have given new impetus to the development of a finite difference analysis procedure that is based on the principle of minimum total potential energy, referred to as "Finite-Difference Energy" method "FDE" [cf. Bushnell Ref. (2)].

A main difficulty in the use of the conventional finite difference method is the incorporation of the boundary conditions.

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Since in the analysis, the differential equation of equilibrium of the system is approximated directly by the difference scheme , it is necessary to satisfy in the differencing both the geometric and the natural boundary conditions. This can be difficult to achieve at arbitrary boundaries [cf. Fayed Ref.(3)], since the topology of the finite difference mesh restricts the form of differencing that can be carried out, and it may be difficult to maintain symmetry properties in the coefficient matrix.

In the FDE method, the displacement derivatives in the total potential energy J of the system are approximated by finite differences ; and the minimum condition of J is used to calculate the unknown displacement parameters. Since the variational formulation is employed , only the geometric boundary conditions need be satisfied in the differencing. Furthermore , symmetry and positive definiteness in the coefficient matrix of the algebraic equations are assured.

As might as well be expected , the FDE is very closely related to "The Displacement Finite Element" method [cf. Bushnell Ref.(4)], and in some cases the same algebraic equations are generated. The specific differences between FEM and FDE lie essentially in the choice of the generalized displacement components and the locations of the nodes that correspond to the generalized displacements.

An advantage of FDE lies in the effectiveness with which the coefficient matrix of the algebraic equations can be generated. This is due to the simple scheme of energy integration employed.

The primary end of the present paper is to give an estimate of error of FDE for a variational class of the fourth order, based on an analytic procedure. This procedure has been developed originally for eigenvalue problems of the general Sturm - Liouville equation [cf. Safwat Ref.(5) and Kurtz et al Ref.(6)].

This error estimate will assess the potential of any finite difference approximation in the FDE method.

2. VARIATIONAL CLASS.

Let the considered variational problem be given by the functional

$$J[\chi(x)] = \frac{1}{2}\int_0^1 (s\chi''^2 - p\chi'^2 + q\chi^2 - 2r\chi)\, dx \tag{1}$$

in which the functional $J[\chi(x)]$ being defined in $C^2[0,1]$, and $s(x)$, $p(x)$, $q(x)$ and $r(x)$ are real analytic functions in the interval $[0,1]$. $J[\chi(x)]$ is subjected to the following constraints

$$\begin{aligned} \chi(0) &= \chi_0 \quad , \quad \chi(1) = \chi_1 \\ \chi'(0) &= \chi'_0 \quad , \quad \chi'(1) = \chi'_1 \end{aligned} \tag{2}$$

Functional (1) are met with frequently in continuum mechanics. As an illustration, consider the deflection w of a beam-column whose length is ℓ that rests on an elastic foundation of modulus k. If EI represents the nonuniform flexural stiffness of the beam in the vertical plane of bending and the beam is subjected to nonuniform inplane load N (taken positive in tension) then the total strain energy in the beam-column is [cf. Donnell Ref.(7) p.70]

$$U = \frac{1}{2}\int_0^{\ell} (EIw''^2 + Nw'^2 + kw^2 - 2pw)\, dx \tag{3}$$

where $p(x)$ is the distributed lateral load intensity. Also, functional (1) can be considered as a prototype to the following functional

$$J[\underline{\chi}(x)] = \frac{1}{2}\int_0^1 \Big(\underline{\chi}''^T[S(x)]\,\underline{\chi}'' - \underline{\chi}'^T[P(x)]\,\underline{\chi}' + \underline{\chi}^T[Q(x)]\,\underline{\chi} - 2\,\underline{r}^T(x)\,\underline{\chi}\Big)\, dx \tag{4}$$

where $\underline{\chi} = \underline{\chi}(x)$ is a column vector of n elements, $[P(x)]$, $[Q(x)]$ and $[S(x)]$ are symmetric square matrices and $\underline{r}(x)$ is a column vector. Such a functional defined by Eq.(4) occurrs in the theory of thin elastic composite shells [cf.Greenberg

3. ERROR ESTIMATE.

Let the derivatives χ' and χ'' be approximated by

$$\chi' = (E - E^{-1})(\chi/2h) \quad , \quad \chi'' = (E - 2 + E^{-1})(\chi/h^2) \tag{5}$$

where E is the displacement operator and h is the mesh length. This approximation is denoted as FDA(1) (Finite difference approximation #1).

Substituting expressions (5) in Eq.(1) and extremizing, yield the difference equation

$$\mathcal{L}^{(1)}\chi - r = 0 \tag{6}$$

where $\mathcal{L}^{(1)}$ is a difference operator correspondent to FDA(1), and it is defined by

$$\begin{aligned}\mathcal{L}^{(1)}(\ldots) = {} & E^{-1}(s/h^4 + p/4h^2)E^{-2}(\ldots) - (E^{-1}+1)(2s/h^4)E^{-1}(\ldots) \\ & + \left[(E^{-1}+E)(s/h^4 - p/4h^2) + (q + 4s/h^4)\right](\ldots) \\ & - (1+E)(2s/h^4)E(\ldots) + E(s/h^4 + p/4h^2)E^2(\ldots).\end{aligned} \tag{7}$$

It is seen that Eq.(6) generates a symmetric system. This yields two merits, namely, reduction in computer memory and secondly, for eigen-analysis, the resulting eigenvalues are real.

To estimate the included error in Eq.(6), one uses the expansion of E operator in terms of the D operator, i.e.,

$$E = 1 + hD + h^2D^2/2 + h^3D^3/6 + h^4D^4/24 + \cdots \tag{8}$$

The substitution of expansion(8) in Eq.(6) leads to a differentail equation with infinite terms that takes the form

$$L_0^{(1)}\chi - r + h^2 L_1^{(1)}\chi + h^4 L_2^{(1)}\chi + \cdots = 0 \tag{9}$$

which satisfy conditions(2) and $L_0^{(1)}$, $L_1^{(1)}$ and $L_2^{(1)}$ are linear differential operators defined by

$$L_0^{(1)} = sD^4 + 2s'D^3 + (s'' + p)D^2 + p'D + q \tag{10.a}$$

$$\begin{aligned}L_1^{(1)} = {} & \frac{s}{6}D^6 + \frac{s'}{2}D^5 + \left(\frac{7}{12}s'' + \frac{p}{3}\right)D^4 + \left(\frac{s'''}{3} + \frac{2}{3}p'\right)D^3 \\ & + \left(\frac{s^{IV}}{12} + \frac{p''}{2}\right)D^2 + \frac{p'''}{6}D.\end{aligned} \tag{10.b}$$

$$L_2^{(1)} = \frac{s}{80}D^8 + \frac{s'}{20}D^7 + \left(\frac{31}{360}s'' + \frac{2}{45}p\right)D^6 + \left(\frac{s'''}{12} + \frac{2}{15}p'\right)D^5$$
$$+ \left(\frac{7}{144}s^{IV} + \frac{p''}{2}\right)D^4 + \left(\frac{s^{V}}{60} + \frac{p'''}{9}\right)D^3 + \left(\frac{s^{VI}}{360} + \frac{p^{IV}}{24}\right)D^2 + \frac{p^{V}}{120}D. \quad (10.c)$$

It is very clear that when h goes to zero , Eq. (9) approaches the Euler equation of Functional (I) . Hence, a solution of Eq. (9) that satisfy conditions (2) gives an analytic representation of the numerical finite difference answers. Since Eq. (9) comprises of infinite terms , a closed form solution seems unfeasible. However, since h is usually small , this suggests the use of perturbation analysis where h^2 is taken as the perturbation parameter.

Let χ be of the form

$$\chi = \varphi + h^2\psi^{(1)} + \cdots . \quad (11)$$

Substituting Eq. (11) in Eq. (9) leads to

$$L_0^{(1)}(\varphi + h^2\psi^{(1)}) - r + h^2 L_1^{(1)}(\varphi + h^2\psi^{(1)}) + \cdots = 0 \quad (12)$$

Equating the coefficients of equal powers of h^2 on both sides of Eq. (12) , one can obtain

$$L_0^{(1)}\varphi - r = 0 \quad (13.a)$$

with $\varphi(0) = \chi_0$, $\varphi(1) = \chi_1$ (13.b)

and $\varphi'(0) = \chi_0'$, $\varphi'(1) = \chi_1'$

$$L_0^{(1)}\psi^{(1)} = -L_1^{(1)}\varphi \quad (14.a)$$

with $\psi^{(1)}(0) = \psi'^{(1)}(0) = \psi^{(1)}(1) = \psi'^{(1)}(1) = 0.$ (14.b)

Clearly, φ is the exact extremal function and from the form of χ given by Eq. (11) , it can be seen that $\psi^{(1)}$ can be interpreted as the first order term in the finite differences results. Thus, the magnitude of $\psi^{(1)}$ is the error estimate of FDE method due to use of FDA (1) .

The second FDA (2) is based on the idea [cf. Stetter Ref. (9)] of using two grids instead of one grid as in FDA (1) . The original grid Γ is associated with another grid - called dual grid - Γ_d whose points are the centres of Γ .

Splitting the functional $J[\chi(x)]$ into two parts, i.e,

$$J_1 = \frac{1}{2}\int_0^1 (s\chi''^2 + q\chi^2 - 2r\chi)\,dx \qquad (15.a)$$

$$J_2 = -\frac{1}{2}\int_0^1 p\chi'^2\,dx \qquad (15.b)$$

Approximating J_1 via grid Γ by $\chi_i'' = (\chi_{i+1} - 2\chi_i + \chi_{i-1})/h^2$ and approximating J_2 via grid Γ_d by $\chi'_{i+\frac{1}{2}} = (\chi_{i+1} - \chi_i)/h$ and extremizing, lead to the following difference equation

$$\mathcal{L}^{(2)}\chi - r = 0 \qquad (16)$$

where the difference operator $\mathcal{L}^{(2)}$ corresponds to FDA (2) and is defined by

$$\begin{aligned}\mathcal{L}^{(2)}(\cdots) = {} & E^{-1}(s/h^4)\,E^{-2}(\cdots) + \left[E^{-1/2}(p/h^2) - (E^{-1}+1)(2s/h^4)\right]E^{-1}(\cdots)\\ & + \left[(E^{-1}+E)(s/h^4) - (E^{-1/2}+E^{1/2})(p/h^2) + q + 4s/h^4\right](\cdots)\\ & + \left[E^{1/2}(p/h^2) - (1+E)(2s/h^4)\right]E(\cdots) + E(s/h^4)E^2(\cdots)\,.\end{aligned} \qquad (17)$$

The equivalent differential equation takes the form

$$L_0^{(2)}\chi - r + h^2 L_1^{(2)}\chi + h^4 L_2^{(2)}\chi + \cdots = 0 \qquad (18)$$

subject to conditions (2), and

$$L_0^{(2)} = sD^4 + 2s'D^3 + (s''+p)D^2 + p'D + q \qquad (19.a)$$

$$L_1^{(2)} = \frac{s}{6}D^6 + \frac{s'}{2}D^5 + \left(\frac{7}{12}s'' + \frac{p}{12}\right)D^4 + \left(\frac{s'''}{3} + \frac{p'}{6}\right)D^3 + \left(\frac{s^{iv}}{12} + \frac{p''}{8}\right)D^2 + \frac{p'''}{24}D \qquad (19.b)$$

$$\begin{aligned}L_2^{(2)} = {} & \frac{s}{80}D^8 + \frac{s'}{20}D^7 + \left(\frac{31}{360}s'' + \frac{p}{360}\right)D^6 + \left(\frac{s'''}{12} + \frac{p'}{120}\right)D^5\\ & + \left(\frac{7}{144}s^{iv} + \frac{p''}{96}\right)D^4 + \left(\frac{s^{v}}{60} + \frac{p'''}{144}\right)D^3 + \left(\frac{s^{vi}}{360} + \frac{p^{iv}}{384}\right)D^2 + \frac{p^{v}}{1920}D\,.\end{aligned} \qquad (19.c)$$

Repeating the same steps carried out in FDA (1), the error estimate $\psi^{(2)}$ is given by

$$L_0^{(2)}\psi^{(2)} = -L_1^{(2)}\varphi \qquad (20.a)$$

with $\psi^{(2)}(0) = \psi'^{(2)}(0) = \psi^{(2)}(1) = \psi'^{(2)}(1) = 0.$ (20.b)

The FDA (3) is suggested as follows. Making use of the two grids Γ and Γ_d, and splitting the functional $J[\chi(x)]$ into two two parts, i.e,

$$J_1 = \frac{1}{2}\int_0^1 s\chi''^2\,dx \qquad (21.a)$$

$$J_2 = \frac{1}{2}\int_0^1 (-p\chi'^2 + q\chi^2 - 2r\chi)\,dx \qquad (21.b)$$

Approximating J_1 via grid Γ by $\chi_i'' = (\chi_{i+1} - 2\chi_i + \chi_{i-1})/h^2$ and J_2 via grid Γ_d by $\chi'_{i+\frac{1}{2}} = (\chi_{i+1} - \chi_i)/h$, $\chi_{i+\frac{1}{2}} = (\chi_{i+1} + \chi_i)/2$ and extremizing, lead to the difference equation

$$\mathcal{L}^{(3)}\chi - r = 0 \tag{22}$$

where the difference operator $\mathcal{L}^{(3)}$ corresponds to FDA(3) and is defined by

$$\begin{aligned}\mathcal{L}^{(3)}(\cdots) = {} & E^{-1}(s/h^4)E^{-2}(\cdots) + \left[E^{-\frac{1}{2}}(p/h^2 + q/4) - (E^{-1}+1)(2s/h^4)\right]E^{-1}(\cdots) \\ & + \left[(E^{-1} + 4 + E)(s/h^4) - (E^{-\frac{1}{2}} + E^{\frac{1}{2}})(p/h^2 - q/4)\right](\cdots) \\ & + \left[E^{\frac{1}{2}}(p/h^2 + q/4) - (1+E)(2s/h^4)\right]E(\cdots) + E(s/h^4)E^{2}(\cdots).\end{aligned} \tag{23}$$

The equivalent differential equation is given by

$$L_0^{(3)}\chi - r + h^2 L_1^{(3)}\chi + h^4 L_2^{(3)}\chi + \cdots = 0 \tag{24}$$

subject to conditions (2), and

$$L_0^{(3)} = sD^4 + 2s'D^3 + (s'' + p)D^2 + p'D + q \tag{25.a}$$

$$\begin{aligned}L_1^{(3)} = {} & \frac{s}{6}D^6 + \frac{s'}{2}D^5 + \left(\frac{7}{12}s'' + \frac{p}{12}\right)D^4 + \left(\frac{s'''}{3} + \frac{p'}{6}\right)D^3 \\ & + \left(\frac{s^{iv}}{12} + \frac{p''}{8} + \frac{q}{4}\right)D^2 + \left(\frac{p'''}{24} + \frac{q'}{4}\right)D + \frac{q''}{8}.\end{aligned} \tag{25.b}$$

$$\begin{aligned}L_2^{(3)} = {} & \frac{s}{80}D^8 + \frac{s'}{20}D^7 + \left(\frac{31}{360}s'' + \frac{p}{360}\right)D^6 + \left(\frac{s'''}{12} + \frac{p'}{120}\right)D^5 \\ & + \left(\frac{7}{144}s^{iv} + \frac{p''}{96} + \frac{q}{48}\right)D^4 + \left(\frac{s^{v}}{60} + \frac{p'''}{144} + \frac{q'}{24}\right)D^3 \\ & + \left(\frac{s^{vi}}{360} + \frac{p^{iv}}{384} + \frac{q''}{32}\right)D^2 + \left(\frac{p^{v}}{1920} + \frac{q'''}{96}\right)D + \frac{q^{iv}}{384}\end{aligned} \tag{25.c}$$

The error estimate $\psi^{(3)}$ is given by

$$L_0^{(3)}\psi^{(3)} = -L_1^{(3)}\phi \tag{26.a}$$

with $\psi^{(3)}(0) = \psi'^{(3)}(0) = \psi^{(3)}(1) = \psi'^{(3)}(1) = 0.$ (26.b)

4. MODEL EXAMPLE.

Consider the following example

$$J[\chi(x)] = \frac{1}{2}\int_0^1 e^{x}(\chi''^2 + \chi'^2 - 2\chi^2 - 2\chi)\,dx. \tag{27}$$

with $\chi(0) = \chi'(0) = \chi(1) = \chi'(1) = 0.$ (28)

The exact extremal function is

$$\varphi = 0.063 \exp(x) + 0.1363 \exp(-2x) + \exp(-x/2) \times \left[0.3007 \cos(\sqrt{3}x/2) + 0.4157 \sin(\sqrt{3}\, x/2)\right] - 1/2. \quad (29)$$

The error estimate ψ takes for every FDA scheme the following expressions :

FDA 1

$$\psi^{(1)} = 0.0034857 \exp(x) + 0.0077023 \exp(-2x) + \exp(-x/2)\left[(-0.011188 + 0.02\, x) \cos(\sqrt{3}\, x/2) - (0.0157905 + 0.0144675\, x) \sin(\sqrt{3}\, x/2)\right]. \quad (30)$$

FDA 2

$$\psi^{(2)} = (0.0242745 - 0.00879\, x) \exp(x) + (0.0246553 + 0.0189305\, x) \exp(-2x) + \exp(-x/2)\left[(-0.0489298 + 0.05\, x) \cos(\sqrt{3}\, x/2) - (0.0688309 + 0.0361685\, x) \sin(\sqrt{3}\, x/2)\right]. \quad (31)$$

FDA 3

$$\psi^{(3)} = 0.0625 - 0.00958 \exp(x) - 0.021019 \exp(-2x) + \exp(-x/2)\left[-(0.0319005 + 0.01\, x) \cos(\sqrt{3}\, x/2) + (-0.0443494 + 0.0072337\, x) \sin(\sqrt{3}\, x/2)\right]. \quad (32)$$

Table 1. Error Estimate.

x	$10^5 \psi^{(1)}$	$10^5 \psi^{(2)}$	$10^5 \psi^{(3)}$
0.0	0.00	0.00	0.00
0.1	3.28	0.20	-6.91
0.2	9.98	0.92	-19.89
0.3	16.40	1.56	-33.25
0.4	20.76	3.41	-40.68
0.5	22.26	6.04	-41.48
0.6	-84.90	4.14	-37.23
0.7	13.83	1.41	-28.07
0.8	8.00	0.91	-15.08
0.9	4.21	0.23	-8.670
1.0	0.00	0.00	0.00

Table 1 shows the values of ψ for different values of x. It can be easily noticed that the accuracy of FDA (2) is the best. In the second place comes FDA(1) while FDA(3) comes the last with respect to accuracy.

5. CONCLUSIONS.

An approach for studying the error estimation of FDE method for a variational class of the fourth order has been presented. Three schemes of central difference approximations are proposed and their accuracy has been evaluated. They have been applied only to one example - that yields an Euler Equation with constant coefficients - which may raise the question "What does happen if they are applied to more complicated variational problems?". In justification, it is valid in many applied cases to approximate a differential equation by a linear one with constant coefficients over short ranges of the independent variable.

Hence , it is recommended that FDA(2) should be used in solving the class of variational problems investigated in the present paper. As for Functional(4) , since an analytic estimation of error is hardly possible, it appears that adopting the results of the prototype Functional(1) is the wise inductive path. Naturally,the final judge will be the numerical experiments.

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