UDC 519.61: 531.2
Original scientific paper
Received: 19.06.2000.

Errors in modelling high order gradient fields using reciprocity based FEM

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SUMMARY

In this paper errors in displacement and stress fields in reciprocity based finite elements are studied in examples of modelling of high order gradient fields using quadratic elements. In the reciprocity based FE formulation Trefftz polynomial functions are used to formulate stiffness matrices by boundary integral equations. This leads to a nonsingular boundary integral formulation in which tractions and displacements on the element boundaries are expressed by the reciprocity relation. The displacements are chosen to be compatible between the elements and weak satisfaction of interelement equilibrium defines the total system of equations in the discretized form. The simple error estimator used in isoparametric elements is compared with the exact error distribution. It is shown that this error estimator is not reliable for elements in which the governing equations are not satisfied inside the element. The results also show the importance of inclusion of boundary conditions for an effective recovery algorithm for stress.

Key words: *error estimator, Trefftz polynomial functions, reciprocity based FEM, high order gradient fields.*

1. INTRODUCTION

The error estimator is an important tool for obtaining solutions with required accuracy over the whole investigated region by remeshing. The quality of the error estimator can save some intermediate steps of the analysis. In most FE formulations we obtain discontinuous stress fields between the elements. This discontinuity is used as a simple error indicator in many FE programs [1]. However, in isoparametric elements, the interelement discontinuity is not the only source of modelling error. The equilibrium equations inside the element are only satisfied in the weak integral sense, and this influences the local error distribution as it is well known [7]. In order to improve the error estimates, the stresses are recovered by using the polynomial interpolation functions for the nodal displacements over the patches of elements [2, 3]. The errors are evaluated as the difference between the stresses obtained from element matrices and those obtained by the stress recovery. Some authors use also equilibrium and boundary conditions to recover more accurate stress fields [4-7].

Our FE formulation is based on the reciprocity principles together with the use of Trefftz-polynomial functions as the test functions (reciprocity fields). Similar ideas were used in Refs. [8-11] and a non-singular BEM formulation can be found in this way. A disadvantage of such a formulation is that it is necessary to use very high degree terms if the region is complicated, and many degrees of freedom are necessary to model the problem with high accuracy. The non-singular boundary element formulation, however, can be used, as it is in our case, to formulate the finite elements (domains in the multi-domain BEM meaning) using similar principles as those used in the hybrid FE formulations [12, 13]. The elements (domains) are connected together based on the satisfaction of the continuity of displacements and on the weak formulation of the inter-domain equilibrium. It is a simple task to find the necessary order of quadrature formulae for accurate numerical integration of all integral terms.

In this contribution we will give the basic principles of the method for elasticity problems. Although the numerical results are shown for 2D problems only, the Trefftz polynomials for 3D problems can be found by numerical procedures, or by algebraic manipulations [14], and thus also the formulation for 3D problems is straightforward. Also the formulations for other field problems of continuum mechanics can be obtained in a similar way.

The accuracy of the reciprocity based FE formulations is studied by modelling high degree (in this paper 6-th degree is used) polynomial fields defined by the Trefftz polynomials (i.e. polynomials satisfying all the governing equations inside the domains). In this way we can study the accuracy of stress as well as displacement fields, and the element behaviour in the parts with small and large field gradients. It is shown that an efficient smoothing procedure can reduce the errors by one order or even more in the fields with high gradients compared to simple averaging of the nodal values in both reciprocity based and isoparametric elements. Reliable local error estimators can be obtained and tested in this way.

2. BETTI'S RECIPROCITY FE FORMULATION

Let us consider the elasticity problem without body forces for simplicity. The boundary displacements $\tilde{u}_i(\tilde{x})$ and tractions $\tilde{t}_i(\tilde{x})$ of each approximated subdomain (element) *'e'* will be related by Betti's reciprocity theorem:

$$\int_{G_e} T_i(\tilde{x})\tilde{u}_i(\tilde{x})dG(\tilde{x}) = \int_{G_e} U_i(\tilde{x})\tilde{t}_i(\tilde{x})dG(\tilde{x}) \quad (1)$$

where $\tilde{x}$ denotes a position field variable, $U_i(\tilde{x})$ are arbitrary displacement fields satisfying the equilibrium conditions inside the element (Trefftz-displacement functions), and $T_i(\tilde{x})$ are corresponding (Trefftz) tractions on the element boundary G_e. The Trefftz functions for displacements can be in polynomial, Legendre, harmonic, Bessel, Hankel, Kupradze's form [15], or they can be the fundamental solutions (in this case also a free term is contained in Eq. (1), as it is known from the BEM formulations [16-19]).

The boundary displacements can be expressed by their nodal values $d^{(j)}$ (the upper index corresponds to the nodal point) and shape functions $N_u^{(j)}$:

$$\tilde{u}_i(x) = N_u^{(j)}(x)d_i^{(j)} \quad \text{or} \quad \{\tilde{u}\} = [N_u]\{d^e\} \quad (2)$$

x is the local co-ordinate of a point on the element boundary, and $\{d^e\}$ is a vector of nodal displacements.

Similarly, tractions can be given by their values $q^{(j)}$ at the nodal points and by corresponding shape functions, $N_t^{(j)}$, as:

$$\tilde{t}_i(x) = N_t^{(j)}(x)q_i^{(j)} \quad \text{or} \quad \tilde{t} = [N_t]\{q^e\} \quad (3)$$

which leads to the matrix form of Eq. (1):

$$[T]\{d^e\} = [U]\{q^e\} \quad (4)$$

where $\{q^e\}$ is a vector of nodal tractions.

Elements of matrices $[T]$ and $[U]$ in Eq. (4) are determined as follows:

$$\begin{aligned} T_{kl} &= \int_{G_e} T^{(k)}(\tilde{x}(x))N_u^{(l)}(x)dG = \\ &= \sum_j T^{(k)}\left(\tilde{x}\left(x^{(j)}\right)\right)N_u^{(l)}\left(x^{(j)}\right)J\left(x^{j}\right)w^{(j)} \\ U_{kl} &= \int_{G_e} U^{(k)}(\tilde{x}(x))N_t^{(l)}(x)dG = \\ &= \sum_j U^{(k)}\left(\tilde{x}\left(x^{(j)}\right)\right)N_t^{(l)}\left(x^{(j)}\right)J\left(x^{(j)}\right)w^{(j)} \end{aligned} \quad (5)$$

where $x^{(j)}$ and $w^{(j)}$ are local co-ordinates and weights in the Gauss quadrature formulae and J is the Jacobian. $T^{(k)}$ and $U^{(k)}$ are tractions and displacements of arbitrary and independent states of the element satisfying all the governing equations.

We will assume that the whole domain will be decomposed into subdomains (elements) and the displacements between the subdomains will be compatible, i.e. the displacements on the element boundaries are common to the neighbouring elements. The tractions, however, will not be in equilibrium between the elements, and so the inter-element equilibrium and natural boundary conditions will be satisfied only in a weak (integral) sense. This is imposed by the variational formulation:

$$\begin{aligned} &\int_{G_t} d\tilde{u}^T(\tilde{t}-\bar{t})dG + \int_{G_i} d\tilde{u}^T\left(\tilde{t}^A-\tilde{t}^B\right)dG = \\ &= \int_{G_e} d\tilde{u}^T\tilde{t}\,dG - \int_{G_t} d\tilde{u}^T\bar{t}\,dG = 0 \end{aligned} \quad (6)$$

In this equation the superscript T denotes transposition, G_i, G_e and G_t are the element boundaries and the domain boundaries with prescribed tractions, respectively. The upper indices A and B denote neighbouring elements with a common boundary. With a bar we denote the prescribed values.

For the purpose of numerical implementation we can write Eq. (6) in the form:

$$\begin{aligned} &\sum_e\sum_j\sum_l N_u^{(k)}\left(x^{(j)}\right)N_t^{(l)}\left(x^{(j)}\right)J\left(x^{(j)}\right)w^{(j)}q^{(l)} = \\ &= \sum_e\sum_i N_u^{(k)}\left(x^{(i)}\right)\bar{t}\left(x^{(i)}\right)J\left(x^{(i)}\right)w^{(i)} \end{aligned} \quad (7)$$

or in the equivalent matrix form:

$$\sum_e\left[M^e\right]\left\{q^e\right\} = \sum_e\left\{p^e\right\} \quad (8)$$

The summations in Eq. (7) relate to elements, Gauss integration points and nodal points, respectively.

From the Eq. (4) we can express the nodal tractions in each element by its nodal displacements as:

$$\left\{q^e\right\} = [U]^{-1}[T]\left\{d^e\right\} \quad (9)$$

and substituting this into Eq. (8) yields:

$$\sum_e\left[M^e\right][U]^{-1}[T]\left\{d^e\right\} = \sum_e\left\{p^e\right\} \quad (10)$$

or:

$$[K]\{d\}=\{p\} \tag{11}$$

This is the resulting system of equations in the discretized form and *[K]* is the global stiffness matrix.

We did not take into account prescribed boundary displacements in the formulas above for the sake of simplicity. Solving the Eq. (11) we obtain the unknown nodal displacements.

In Eq. (9), the number of Trefftz functions (arbitrary states of the element) has to be equal to, or greater than the number of d.o.f. in displacements in order to derive a unique solution.

Similarly, for the unique solution of the inter-element equilibrium (in the weak sense) the number of components of the element displacement vector should be equal to, or greater than, the number of components of its nodal tractions.

3. STRESS EVALUATION

Having obtained the nodal displacements from Eq. (11) the tractions at nodal points for each element can be computed from the Eq. (9).

The stresses were obtained in three ways:

(1) The stresses in the corner points of elements are obtained from the element tractions. The stresses on the element boundaries are calculated in local coordinates (normal and tangent components): Two components for 2D (normal and shear component) and three components in 3D are identical with the tractions (transformed into the corresponding directions) [16]. Let t_s, t_t and t_n be the traction components in two orthogonal directions, *s* and *t* and in the normal direction, respectively, on the element boundaries in the local co-ordinates. The other components of stress can be found from strains obtained from the boundary displacement fields.

In 2D we have:

$$s_{nt}=t_t \qquad s_{nn}=t_n \qquad s_{tt}=\frac{1}{1-n}\left(nt_n+2Ge_{tt}\right) \tag{12}$$

for plane strain (*n*=n/(1+n)* for plane stress) state and:

$$\begin{aligned} &s_{sn}=t_s \qquad s_{tn}=t_t \qquad s_{nn}=t_n \qquad s_{st}=2Ge_{st} \\ &s_{ss}=\frac{1}{1-n}\left[nt_t+2G\left(e_{ss}+ne_{tt}\right)\right] \\ &s_{tt}=\frac{1}{1-n}\left[nt_n+2G\left(e_{tt}+ne_{ss}\right)\right] \end{aligned} \tag{13}$$

for 3D problems, where *G* is the shear modulus. The strains e_{ss}, e_{tt}, e_{st} have to be computed from the displacements at the element nodal points, and the corresponding shape functions on each side of the element separately by the standard methods known from FEM or BEM formulations.

(2) The stresses are obtained from the Trefftz-stress polynomials which correspond to the Treffts displacement functions. These functions are determined from the nodal displacements using a Least Square (LS) numerical procedure similar to that described below.

(3) The stress field is computed by using nodal displacements of the elements and known tractions (prescribed loads) on the boundaries for the definition of Trefftz polynomials for displacements and stresses.

Also, continuous stress fields can be obtained using the Moving Least Square (MLS) techniques from displacements and tractions at the nodal points over some patches of nodes. Similar ideas have been used in [4, 20]. We assume the displacement field (at a field point *x*), *{u(x)}*, is given in the form:

$$\{u(x)\}=[U(x)]\{c\} \tag{14}$$

where *[U(x)]* is a matrix of Trefftz-displacement-functions and *{c}* is the vector of unknown coefficients. If Trefftz polynomials are used for the Trefftz- functions, we can easily express strain and stress fields from displacements (14). The stress field can be written then as:

$$\{s\,(x)\}=[S(x)]\{c\} \tag{15}$$

where the matrix of Trefftz-stress-functions *[S(x)]* is derived from the matrix *[U(x)]*. Similarly, we can express Trefftz-tractions as:

$$\{t(x)\}=[T(x)]\{c\} \tag{16}$$

In this approximation we use the full Trefftz polynomials of the chosen degree and the unknown coefficients *{c}* are computed by LS method from:

$$\begin{aligned} &\sum_i w_i^d\left([U(x_i)]\{c\}-\{d_i\}\right)^2+ \\ &+\sum_i w_i^t\left([T(x_i)]\{c\}-\{t_i\}\right)^2=min \end{aligned} \tag{17}$$

where $\{d_i\}$ and $\{t_i\}$ are the displacements and tractions at the nodal points in a domain of influence, and w_i^d and w_i^t are corresponding weighting functions necessary for the dimensionality.

The accuracy of the last method is much higher than the other two as was shown in [21].

4. HIGH DEGREE TREFFTZ POLYNOMIAL FIELDS IN ELASTICITY PROBLEMS

For the sake of investigation of modelling errors and error estimation in FEM formulations we studied the problems on the models of a simple quadrilateral domain with displacement boundary conditions corresponding to the problem described by high degree Trefftz (we chose the 6-th degree) polynomials. Young modulus equal to 1000 MPa and Poisson ratio equal to 0.3 were chosen in the calculations. The domain was approximated by eight noded quadrilateral quadratic (isoparametric serendipity) elements in ADINA, and by the same shape and the same order of approximation was used for the reciprocity based elements. The displacements of the nodal points on the domain boundary were prescribed according to the exact Trefftz solution, and so the exact errors in both displacement and stress fields could be studied.

Figure 1 shows the deformed region as defined by the test 6-th degree Trefftz displacement polynomials. The mesh and contours of the displacement (magnitudes of the vector field values), and von Mises stress fields of the test fields are given in Figures 2 and 3, respectively. In all these and following Figures, as well, the maximal values of corresponding field variables in the region are given, so that we can obtain information about relative errors, as well.

Errors in the calculated fields of the von Misses stress obtained from the quadratic isoparametric serendipity elements are given in Figure 4, and those obtained by the reciprocity based FE are shown in Figure 5. The mesh of 10 by 10 elements was used in both cases. Corresponding displacement fields are given in Figures 6 and 7.

The informations like those indicated in Figures 4 to 7 cannot be obtained for general problems. Instead some error estimators are used in the stress recovery phase [2-7]. One of the simplest error estimators is that used in many commercial programs [1] based on the jumps in the stress fields between neighbour elements. However, if elements are used in which the equilibrium equations are not satisfied inside the elements (in a strong sense), then such error estimators are not reliable as we can see from Figure 8. We can obtain not only underestimated errors, but also incorrect distributions of errors (see Figures 4 and 8 for comparisons).

The errors in displacement field are given in Figure 9 with both prescribed boundary displacements (Figure 9a) and prescribed boundary tractions (Figure 9b). From this figures we can see the behaviour of exact errors in the quadratic elements. Obviously, the discontinuities of the first derivative of the

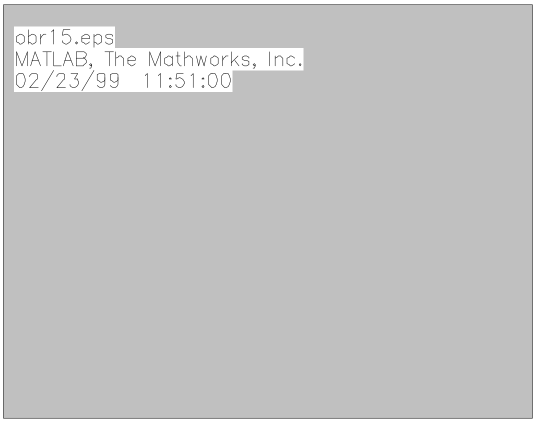
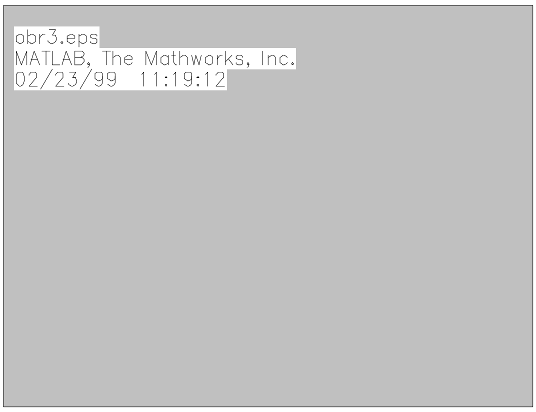


Fig. 1 Deformed region described by the test Trefftz polynomials of 6th degree (Max. 4.0136)

a)



b)

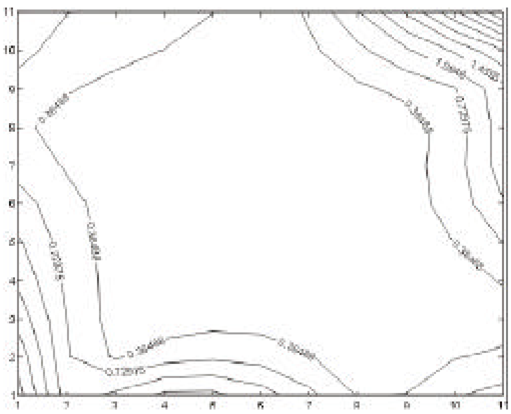
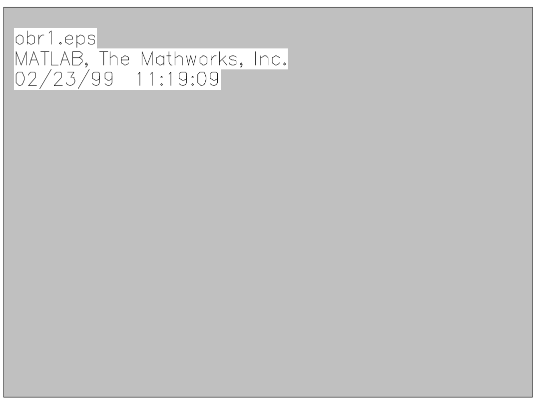


Fig. 2 Mesh (a) and contours (b) of test displacements given by Treffts displacement polynomials of 6th degree (Max. 4.0136)

a)



b)

Fig. 3 Mesh (a) and contours (b) of test von Mises stresses defined by Trefftz stress polynomials of 6th degree (Max. 1.4488e+4)

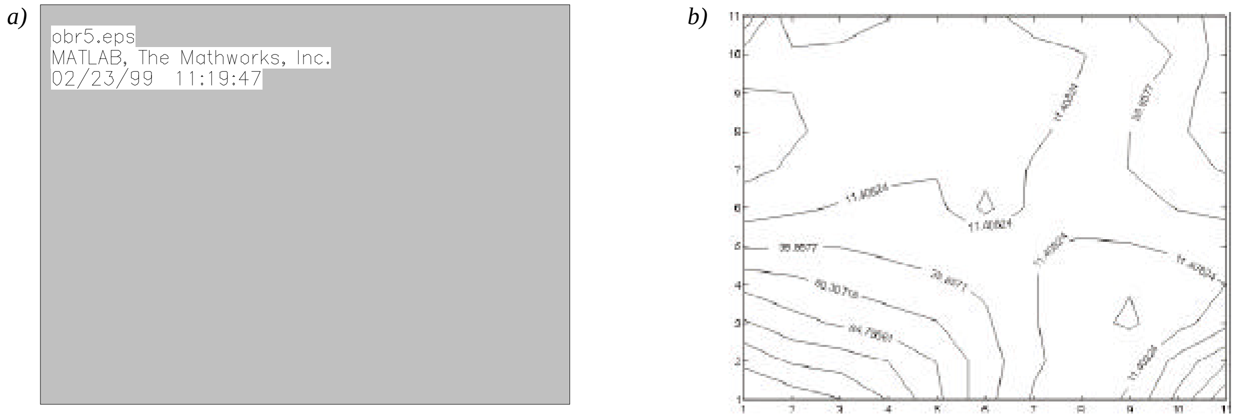


Fig. 4 Mesh (a) and contours (b) of errors in von Mises stress field computed from the quadratic isoparametric mesh of elements (Max. 182.5544)

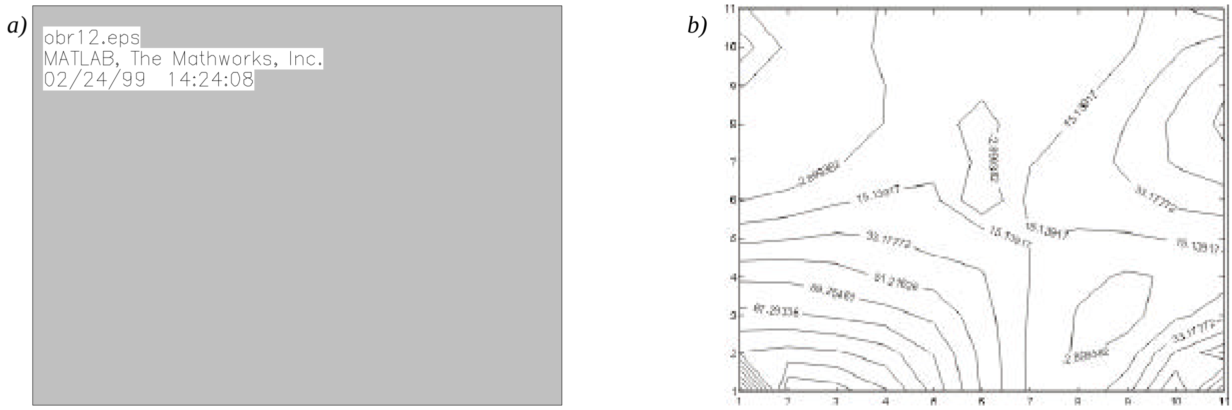


Fig. 5 Mesh (a) and contours (b) of errors in von Mises stress field computed from the quadratic reciprocity based 10x10 elements (Max. 177.4861)

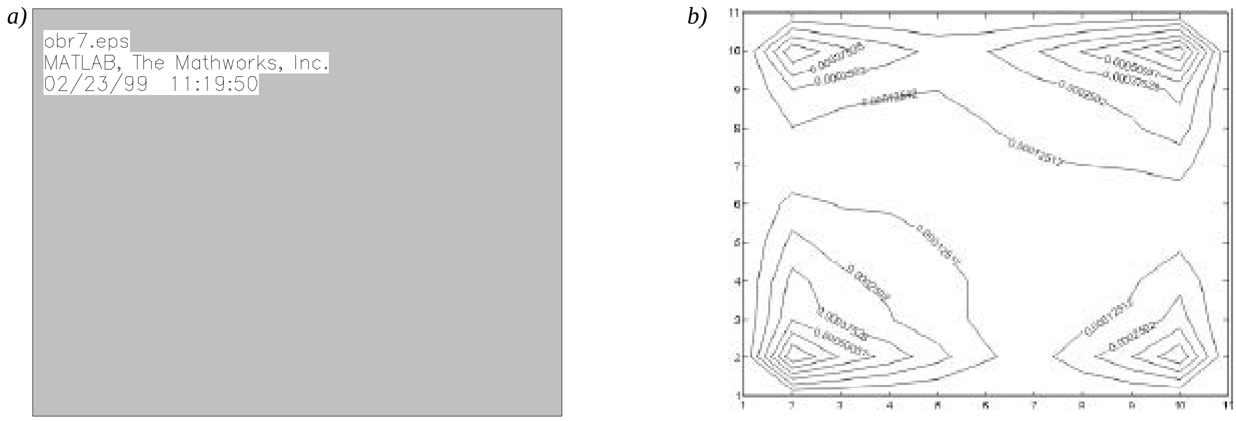


Fig. 6 Mesh (a) and contours (b) of errors in displacement field computed from the quadratic isoparametric elements (Max. 8.7562e-4)

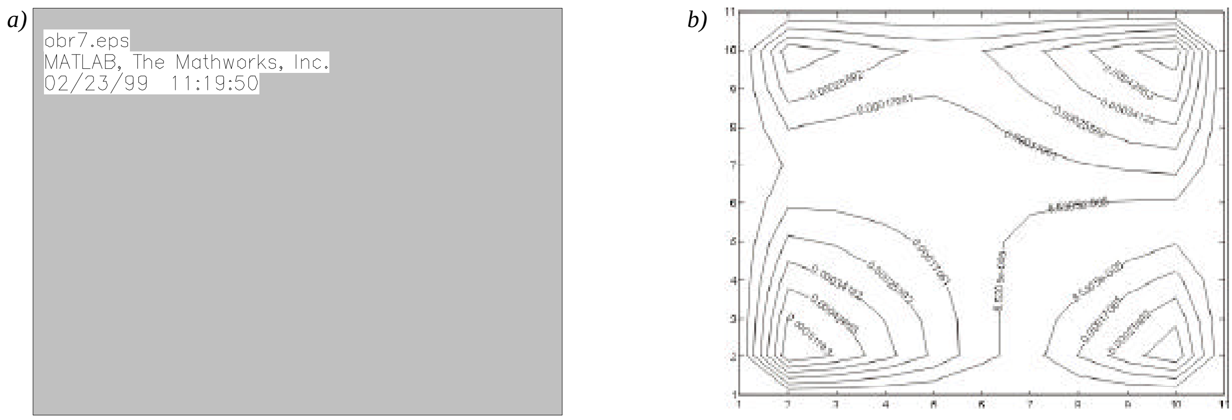


Fig. 7 Mesh (a) and contours (b) of errors in displacement field computed from the quadratic reciprocity based elements (Max. 5.9714e-4)

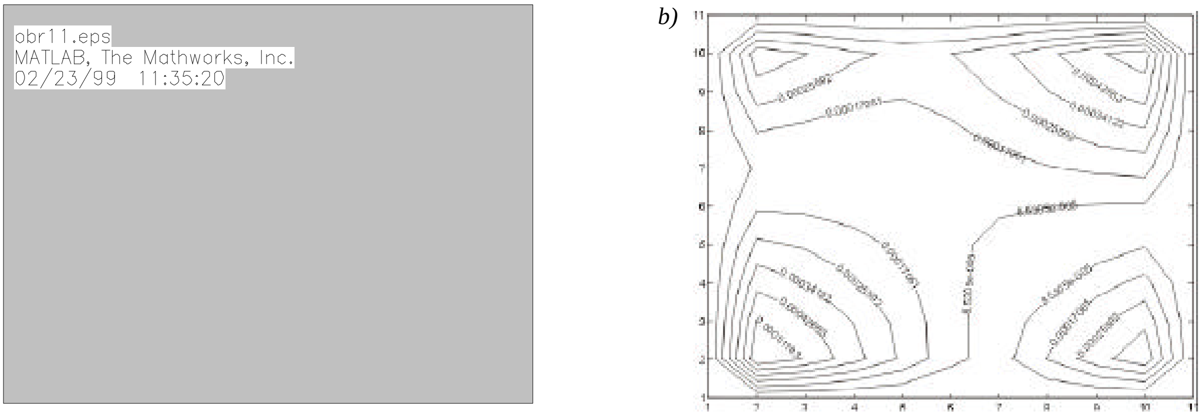


Fig. 8 Error field estimated from interelement stress incompatibilities by isoparametric displacement FE formulation

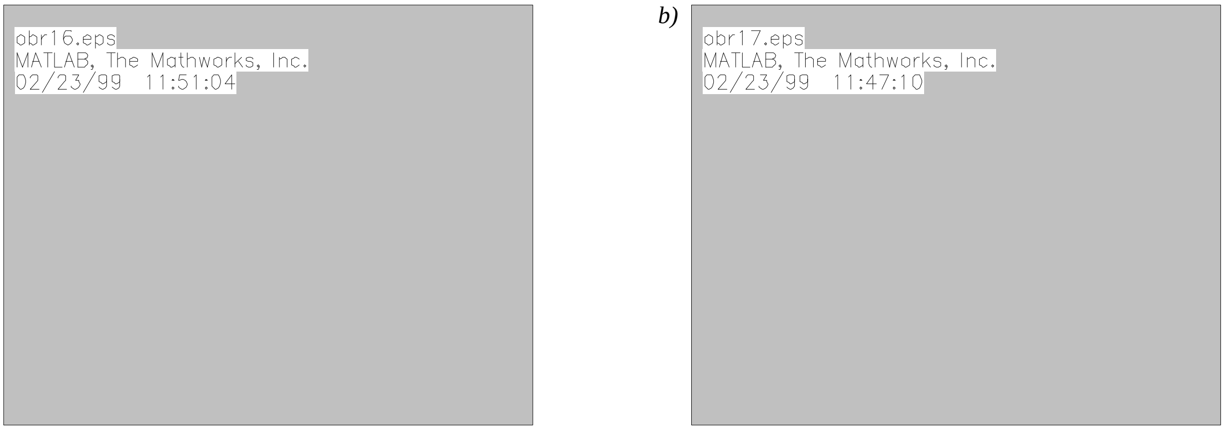


Fig. 9 FE mesh distored by displacement errors with prescribed displacement (a) and tractions (b), respectively

displacement fields (apparent slope discontinuities along the element boundaries are caused by course graphics) are basis of the stress jumps between the elements and so, the roughness of displacement errors (not the total errors in displacements) and errors in stress fields are closely related. Comparing the Figures 9a and 9b, we can see that the roughness of both fields is comparable, if we exclude the outer rows of elements. This shows, how important is to include the static boundary conditions in the evaluation of stress fields on the parts of the boundaries with prescribed tractions. For comparison we give only some maximal values of the field variables as follows:

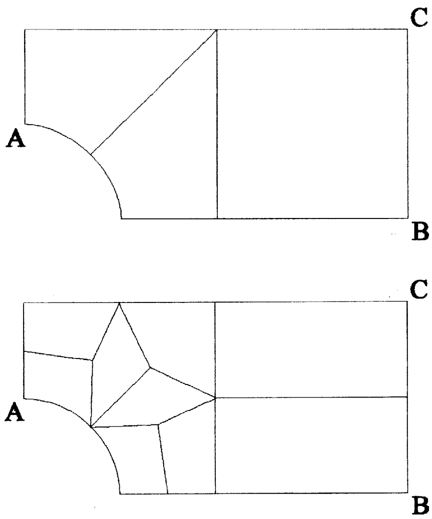
Von Mises stress:	14488.
Error in tractions:	224.
Error in the averaged stress:	145.
Error in the smoothed stress:	21.

The smoothed stresses were obtained using MLS techniques using quadratic Trefftz interpolation polynomials with the Domain of Influence of the same size as the diagonal of the elements, and using the known boundary tractions in the Point of Interest (POI) when the POI was on the boundary of the domain.

In the last example the band with hole was modelled by the reciprocity based FEM. Because of the symmetry only a quarter of the problem was modelled. The stresses in the point A for 3 and 9 element models (Figure 10) compared with analytical solution for infinite band and with FEM solution obtained with very fine isoparametric model (643 quadratic elements) are:

3 elements reciprocity:	4.15
9 elements reciprocity:	4.31
463 elements isoparametric:	4.36
analytic solution:	4.3

a)



b)

Fig. 10 FE models for a band with hole: (a) 3 element model, and (b) 9 element model

The overall convergence properties can be studied on the behaviour of primary (displacement) field and it is documented on the total deformation of the region (points B and C in Figure 10). Vectors of displacements in the points B and C are given in the first and second column in the following table and compared with isoparametric 463 element solution:

3 elements:	0.006109	0.005437
9 elements:	0.005911	0.005378
463 elements:	0.005825	0.005382

5. CONCLUSIONS

The objective in this paper was to present errors in FEM modelling. If the difference between the smoothed fields obtained by averaging in the nodal points of neighbour elements and the values obtained from element equations are taken as the error estimators, we have shown that such error estimators not only underestimate the errors, but also give different error fields from their exact values. The source of this effect is that the interelement incompatibility in tractions alone cannot correctly introduce the approximation errors. If the same procedure is used for elements defined on the basis of reciprocity, when the only equations, which are satisfied in the weak sense, are the interelement equilibrium equations, then the traction incompatibility gives the upper boundaries for errors in stress fields. However, if smooth stress fields are obtained from nodal displacements and boundary tractions using Trefftz polynomial interpolating functions, then the errors in stress field are lower than those indicated by the jumps in tractions in the neighbour elements.

The exact errors were obtained when the Trefftz polynomials of higher degree were used for test functions. Both geometric and static boundary conditions were examined. This type of test showed the importance of taking into account the boundary conditions in the postprocessing (stress recovery) stage. The errors in the recovered stress field are one order lower in the example with higher gradients than those obtained by simple averaging of their nodal values.

ACKNOWLEDGEMENT

This work was partly supported by Grant No. 1/3278/96 of the Slovak Grant Agency for Science.

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POGREŠKE U MODELIRANJU GRADIJENTNIH POLJA VISOKOG STUPNJA UPORABOM RECIPRO^NO UTEMELJENE METODE KONA^NIH ELEMENATA

SA@ETAK

U ovom se radu pogreške pomaka i polja naprezanja u recipro~no utemeljenim kona~nim elementima prou~avaju na primjerima modeliranja gradijentnih polja visokog stupnja, koriste}i kvadratne elemente. U recipro~no utemeljenoj formulaciji kona~nih elemenata Trefftz-ove polinomne funkcije koriste se za formuliranje matrice krutosti pomo}u rubnih integralnih jednad`bi. To dovodi do nesingularne rubne integralne formulacije u kojoj se deformacije i pomaci na granicama elemenata izra`avaju pomo}u odnosa recipro~nosti. Pomaci su odabrani tako da budu kompatibilni izme|u elemenata, a nejako zadovoljenje ravnote`e me|u elementima definira cijeli sustav jednad`bi u diskretiziranom obliku.

Jednostavni ocjenjiva~ pogreške koji se koristi u izoparametrijskim elementima uspore|uje se s to~nom distribucijom pogreške. Vidi se da ovaj ocjenjiva~ pogreške nije pouzdan za elemente u kojima nisu zadovoljene vode}e jednad`be unutar elemenata. Rezultati tako|er pokazuju va`nost uklju~ivanja rubnih uvjeta zbog efikasnog obnavljanja algoritma naprezanja.

Klju~ne rije~i: *ocjenjiva~ pogre{ke, Trefftz-ove polinomne funkcije, recipro~no utemeljena MKE, gradijentna polja visokog stupnja.*