Trefftz-polynomial reciprocity based FE formulations

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The paper contains a general procedure for obtaining of Trefftz polynomials of arbitrary order for 2D or 3D problems by numerical or analytical way. Using Trefftz polynomials for displacement and tractions the unknown displacements and tractions are related by non-singular boundary integral equations. For a multidomain (element) formulation we suppose the displacements to be continuous between the sub-domains and the tractions are connected in a weak (integral) sense by a variational formulation of inter-element equilibrium. The stiffness matrix defined in this way is nonsymmetric and positive semi-definite. The finite elements can be combined with other well known elements. The form of the elements can be, however, more general (the multiply connected form of the element is possible, transition elements which can be connected to more elements along one side are available). It is also very easy and simply possible to assess the local errors of the solution from the traction incompatibilities (the inter-element equilibrium, which is satisfied in a weak sense only, is the only incompatibility in the solution of the linear problem). The stress smoothing is a very useful tool in the post-processing stage. It can improve the accuracy of the stress field by even one order or more comparing to the simple averaging, if the stress gradients in the element are large. Also the convergence of the so obtained stress field increases. The examples with high order gradient field and crack modelling document the efficiency of this FEM formulation. The extension to the solution of other field problems is very simple.

1. Introduction

The Betti's reciprocity enables to relate the unknown state of boundary displacements of a solid to its tractions by relating the reciprocal work of the known and unknown states of the solid. Applications of these principles are well known from the boundary element method (BEM) [1, 3, 7] in which the known states of the solid are defined by the fundamental (Kelvin) solution and lead to boundary integral equations (BIE) with weakly or strongly singular kernels. In the stress evaluation or in some formulations also hyper-singular kernels and in thin walled problems quasi-singular kernels are to treat. Special technique are necessary to get required accuracy in all such problems.

If polynomial functions, which satisfy all governing equations (the Treffz functions) [16, 27, 29] are used in the Betti's reciprocity formulations, the BIE are regular and the order of quadrature formulas necessary for integration is simply estimated. The Trefftz functions are obtainable by analytical (using symbolical calculation) or numerical ways for both 2D and 3D problems as it is shown in the first part of our paper.

Different formulations using the Trefftz functions are known, e.g. the direct Trefftz methods [9, 10, 13–15] or the hybrid-Trefftz-FEM [12, 17, 20]. In our formulation, the direct Trefftz method is realized to the multi-domain solution and some basic principles of both mentioned groups are used.

The Trefftz functions in the Betti's reciprocity formulations play similar role as the weighting (or test) functions by variational formulations [2, 30], i.e. we need to have enough such functions to compute all degrees of freedom of the approximate functions. If the problem is complicated, then high order Trefftz polynomials are required in order to have enough independent terms for the reciprocity relations. The higher order Trefftz polynomials, however, contain too many terms and the procedure become less effective. In our formulations, we use a multi-domain (element) form of the solution in which the tractions and displacements inside each sub-domain are related by the

Betti's reciprocity and the variational formulation is used to connect the elements together. The displacements between the elements are supposed compatible and the inter-element equilibrium (continuity of tractions) is satisfied in a weak (integral) sense only, similarly, as it is by the hybrid FEM [12, 17, 20]. For the elements defined in this form, lower order polynomials suffice to define the unknown coefficients and the solution is still very effective and the accuracy is higher than by classical FEM formulations [2, 30].

The element stiffness matrices defined in this form are symmetric (also for one element region). In this way the symmetric BEM formulation can be obtained also for classical (singular) BEM formulations. Another kind of symmetric BEM's is obtained by the symmetric Galerkin BEM formulations [5, 6, 8, 23]. Our formulation enables very simply to combine the elements with other displacement FEM formulation. Moreover, the elements can have more general form, e.g. we can simply define the transition elements, because we can define finite elements having two or more boundary elements on one side in reciprocity relations. Also classical, singular formulations can be used for the sub-domain definitions in connection with our variational formulation.

The gradients of the primary (displacement) fields required for the computation of strains and stresses are incompatible between the elements. The smoothed fields are obtainable in the post-processing (stress or strain recovery procedures) [4, 11, 24, 25, 28, 31]. When Moving Least Squares (MLS) technique using the Trefftz polynomial approximation is employed, a dramatic improvement of accuracy is achieved. It is shown that the rate of accuracy improvement of smoothed stress field increase with the mesh refining similarly as that of displacements, while the accuracy improvement of simple averaged field is slower than that by displacements.

A reliable error estimator is the inter-element traction incompatibility and the incompatibility between the given and computed tractions on the domain boundaries [19, 21, 22].

Two examples show the efficiency of the present formulation. The first one models the stress and displacement fields with large gradients described by the Trefftz polynomials of higher (6-th) order so that exact errors could be examined. The second example solves the problem with cracks.

2. GENERATION OF TREFFTZ (T-)POLYNOMIAL FUNCTIONS IN 3D

We will assume an isotropic linear elastic solid without body forces. We do not suppose the body forces for simplicity. The displacement field which describes its behaviour under static loading conditions have to satisfy the equilibrium equations which are expressed by Lame–Navier equations

$$(\lambda + \mu)u_{j,ij} + \mu u_{i,jj} = 0 \tag{1}$$

where i, j = 1, 2, 3 for 3D problems. u_i is the *i*-th component of the displacement field with subscripts after comma denoting partial derivatives in corresponding co-ordinate component direction and with summation appointment after repeated indices. λ and μ are Lame constants expressed by Young's modulus, E and Poisson's ratio ν ,

$$\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)} , \qquad \mu = \frac{E}{2(1+\nu)} .$$
 (2)

We will consider the polynomial approximation of the displacement field,

$$\left\{\begin{array}{c} u_1 \\ u_2 \\ u_3 \end{array}\right\} = \left[\begin{array}{ccc} \mathbf{P}(\mathbf{x}) & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{P}(\mathbf{x}) & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{P}(\mathbf{x}) \end{array}\right] \left\{\begin{array}{c} \mathbf{c}^{(1)} \\ \mathbf{c}^{(2)} \\ \mathbf{c}^{(3)} \end{array}\right\}, \tag{3}$$

where P(x) is full polynomial of the *n*-th order

$$\mathbf{P}(\mathbf{x}) = \begin{bmatrix} 1 & x_1 & x_2 & x_3 & \dots & x_1^n & x_1^{n-1} x_2 & \dots & x_2 x_3^{n-1} & x_3^n \end{bmatrix}$$
(4)

and $\mathbf{c}^{(j)}$ is a vector of unknown coefficients.

The equilibrium equation (1) contains the second derivatives of the displacements. Thus, the terms of the zeroth and first order satisfy the homogeneous equation (1), i.e. that without the body forces. However, the higher order polynomials cannot be arbitrary to satisfy the Eq. (1). If we conveniently split (3) into the form

where **B** contains as many terms of each order as there are polynomial terms of two order lower (because the equilibrium equations will be two order lower polynomials obtained by differentiation of approximation displacements field). So for example the third order terms

$$\frac{x_1^2 x_2}{x_1 x_2^2} \frac{x_1^2 x_3}{x_1 x_2 x_3} \frac{x_1 x_3^2}{x_2^2 x_3}$$

$$\frac{x_2^3}{x_2^2 x_3} \frac{x_2^2 x_3}{x_3^2} \frac{x_3^3}{x_3^3}$$

$$(6)$$

will be split so that the upper three terms will be contained in $\mathbf{B}^{(1)}$ and the lower part terms in $\mathbf{A}^{(1)}$. Cyclically changing the components indices we will obtain the terms for $\mathbf{B}^{(j)}$ and $\mathbf{A}^{(j)}$ (j=2,3).

To satisfy the equilibrium (1) we differentiate $\mathbf{B}^{(j)}$ and $\mathbf{A}^{(j)}$ and set into (1) and obtain the relation

$$[\mathbf{M}(x_i)] \{\mathbf{b}\} + [\mathbf{N}(x_i)] \{\mathbf{a}\} = \{\mathbf{0}\}.$$
 (7)

Now the vector **b** contains dependent coefficients which have to be expressed through the (independent) coefficients **a** in order to satisfy the equilibrium equations in the strong sense.

The problem can be solved for each order separately. It can be done symbolically (e.g. in MAPLE) or numerically. In the last case we choose arbitrary as many points as we have the dependent terms and get (7) in the form

$$[\mathbf{M}^{(j)}(x_i)] \{\mathbf{b}\} = -[\mathbf{N}^{(j)}(x_i)] \{\mathbf{a}\}$$
(8)

and compute b as

$$\{ \mathbf{b} \} = - [\mathbf{M}^{-1}] [\mathbf{N}] \{ \mathbf{a} \}$$
 (9)

With this we obtain T-polynomial displacements (i.e. displacements satisfying the governing equations in the whole domain) in the form

$$\{ \mathbf{U} \} = ([\mathbf{A}(x_i)] - [\mathbf{B}(x_i)][\mathbf{M}]^{-1}[\mathbf{N}]) \{ \mathbf{a} \} = [\mathbf{U}(x_i)] \{ \mathbf{a} \}$$
(10)

Each column of the matrix **U** in (10) introduces a T-displacement function and the rows are corresponding components. The points have to be conveniently spaced so that the matrix **M** will be not singular. Note, that the number of T-functions which can be derived in this form is 2n + 1 for 2D problems and $(n + 1)^2$ T-functions for 3D problems, where n is the polynomial order.

From the T-displacements corresponding T-stresses are obtained by differentiating (10) and setting into (11),

$$\Sigma_{ij} = \mu(U_{i,j} + U_{j,i}) + \lambda \delta_{ij} U_{k,k} \tag{11}$$

and corresponding T-tractions on the boundaries with the outer normal n_j

$$T_i = \Sigma_{ij} n_j \tag{12}$$

where δ_{ij} is the Kronecker delta.

3. RECIPROCITY BASED FEM (MULTI-DOMAIN SYMMETRIC BEM) FORMULATION

Let us consider the elasticity problem without body forces again. The boundary displacements $u_i(x)$ and tractions $t_i(x)$ of each approximated sub-domain (element) will be related by the Betti's reciprocity theorem [1, 3, 7],

$$\int_{\Gamma_e} T_i(x) u_i(x) \, \mathrm{d}\Gamma(x) = \int_{\Gamma_e} U_i(x) t_i(x) \, \mathrm{d}\Gamma(x). \tag{13}$$

x denotes a field variable, $U_i(x)$ and $T_i(x)$ are corresponding T-(displacement and traction) functions on the element boundaries Γ_e defined in the previous chapter, i.e. by the columns of the matrix $[U(x_i)]$ in Eq. (10) and the tractions defined by Eq. (12). This equation relates the quantities of one state to the other (known) quantities (introduced by Trefftz functions) of the same elastic body.

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

$$u_i(\xi) = N_u^{(j)}(\xi) d_i^{(j)} \quad \text{or} \quad \mathbf{u} = \mathbf{N}_u \mathbf{d}^e.$$
 (14)

 ξ is a local co-ordinate of a point on the element boundary.

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

$$t_i(\xi) = N_t^{(j)}(\xi) q_i^{(j)} \quad \text{or} \quad \mathbf{t} = \mathbf{N}_t \mathbf{q}^e$$
 (15)

which leads to the matrix form

$$\mathbf{Td}^e = \mathbf{Uq}^e. \tag{16}$$

The curved surfaces are approximated by isoparametric elements, however, the same shape functions are used for approximation of normal direction from its nodal values as there are used for coordinates (Eq. (14)). In this way we have incompatibility between the normal direction defined by shape functions and that defined from its nodal values. The normal directions are defined to be continuous in this way (we use this formulation instead of using spline approximation). This simplifies also the smoothing process in the post-processing stage (see below).

Elements of matrices T and U are

$$T_{kl} = \int_{\Gamma_e} T^{(k)}(x(\xi)) N_u^{(l)}(\xi) d\Gamma = \sum_j T^{(k)} \left(x(\xi^{(j)}) \right) N_u^{(l)}(\xi^{(j)}) J(\xi^{(j)}) w^{(j)}, \tag{17}$$

$$U_{kl} = \int_{\Gamma_e} U^{(k)}(x(\xi)) N_t^{(l)}(\xi) d\Gamma = \sum_j U^{(k)}(x(\xi^{(j)})) N_t^{(l)}(\xi^{(j)}) J(\xi^{(j)}) w^{(j)},$$
(18)

where $\xi^{(j)}$ and $w^{(j)}$ are co-ordinates and weights in the Gauss quadrature formulas, respectively, and J is the Jacobian.

Equation (13) is a boundary integral equation and it is regular in contrary to the use of fundamental solutions, in which case it is singular. The advantage of the non-singular formulation is its both simpler numerical evaluation of integral terms (comparing to computing the strong, weak, hyper-, or quasi-singular integrals [1, 3, 7]) and simpler estimation of required numerical integration order for its evaluation with required accuracy. The drawback of this formulation is the increasing number of polynomial terms with increasing degree of approximation of the domain variables (the number of Trefftz functions must be sufficient in order that the solution is unique, i.e. we must have as many equations as many degrees of freedom in the element). These drawbacks can be overcome by using multi-domain (element) formulation. Also the classical singular, hyper-singular, or other BEM formulations can be used for (13) in connection with the multi-domain form of the solution.

The combinations of the different formulations in order to gain advantages of corresponding forms are possible, too.

We will further assume that the whole domain will be decomposed into sub-domains (elements) and the displacements between the sub-domains will be compatible. The tractions, however, will be incompatible between the elements and so the inter-element equilibrium and natural boundary conditions will be satisfied only in a weak (integral) sense using the variational formulation

$$\int_{\Gamma_t} \delta u^T (t - \bar{t}) d\Gamma + \int_{\Gamma_t} \delta u^T (t^A - t^B) d\Gamma = \int_{\Gamma_t} \delta u^T t d\Gamma - \int_{\Gamma_t} \delta u^T \bar{t} d\Gamma = 0$$
(19)

where Γ_i and Γ_t are the inter-element boundaries and the element boundaries with prescribed tractions, respectively. A and B denote the neighbouring elements. With a bar we denote the prescribed values.

Equation (18) in the discretized form is

$$\sum_{e} \sum_{j} \sum_{l} N_{u}^{(k)} \left(\xi^{(j)} \right) N_{t}^{(l)} \left(\xi^{(j)} \right) J \left(\xi^{(j)} \right) w^{(j)} q^{(l)} = \sum_{e} \sum_{i} N_{u}^{(k)} \left(\xi^{(i)} \right) \bar{t} \left(\xi^{(i)} \right) J \left(\xi^{(i)} \right) w^{(i)}$$

$$(20)$$

or, in equivalent matrix form,

$$\sum_{e} \mathbf{M}^{e} \mathbf{q}^{e} = \sum_{e} \mathbf{p}^{e} \tag{21}$$

The summations in (20) relate to elements, Gauss integration nodes and nodal points, respectively. From Eq. (16) we have

$$\mathbf{q}^e = \mathbf{U}^{-1} \mathbf{T} \mathbf{d}^e \tag{22}$$

and substituting this into eq.(20) yields

$$\sum_{e} \mathbf{M}^{e} \mathbf{U}^{-1} \mathbf{T} \mathbf{d}^{e} = \sum_{e} \mathbf{p}^{e} \tag{23}$$

or

$$Kd = p (24)$$

where K is the global stiffness matrix.

From (18) and (19) we can see that the r.h.s. is defined exactly as it is known from the displacement FEM formulations. The element stiffness matrix is symmetric and assembled into the global stiffness matrix also in the same way. Thus, the whole formulation can be arbitrarily combined with sub-domains or element defined by FEM and/or BEM principles as mentioned above.

4. THE STRESS RECOVERY PHASE

Having obtained the nodal displacements from Eq. (23), the tractions in nodal points in each element/sub-domain can be computed from the Eq. (21). The stresses in the corner points of elements can be calculated directly from tractions. Both tractions and stresses are incompatible between the elements. Smooth stress fields can be obtained by more ways. The simplest one is by averaging the nodal values in corresponding neighbour elements [18].

Much more accurate continuous stress fields can be obtained using the Moving Least Squares (MLS) techniques from the nodal displacements and known tractions on the domain boundaries in the nodal points closest to the corresponding point of interest.

We will consider the displacement field (in a field point x), $\mathbf{u}(x)$, given in the form

$$\mathbf{u}(x) = \mathbf{U}(x) \mathbf{a}$$
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where $\mathbf{U}(x)$ is a matrix of T-displacement functions and \mathbf{a} is the vector of unknown coefficients. The stress field is then given by

$$\sigma(x) = \Sigma(x)$$
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Similarly, we can express T-tractions as

$$\mathbf{t}(x) = \boldsymbol{\sigma}(x) \,\mathbf{n}(x) = \mathbf{T}(x) \,\mathbf{a} \tag{27}$$

In this approximation we are to use the full T-polynomials of chosen order and the unknown coefficients **a** are computed by the Least Square (LS-) method from

$$\sum_{I} (\mathbf{U}_{IJ}(x_I) \, \mathbf{a}_J - \mathbf{d}_I)^2 = \min, \tag{28a}$$

$$\sum_{K} (\mathbf{T}_{KJ}(x_K) \, \mathbf{a}_J - \mathbf{t}_K)^2 = \min, \tag{28b}$$

where d_I and t_K are the displacements in the nodal points and tractions in the points with prescribed boundary tractions, respectively. U_{IJ} is the J-th T-displacement function for the I-th nodal component and T_{KJ} is the J-th T-traction function for the K-th traction component in the boundary point. The displacements are considered in the nodal points of the patch of those nodes with distance smaller than prescribed value from the point of interest. Splitting the vector of the unknown coefficients \mathbf{a} and the matrices of T-functions \mathbf{U} and \mathbf{K} in Eq. (27) in convenient way we solve the problem (27) in the form

$$\mathbf{U}_{11}^{T} \, \mathbf{U}_{11} \, \mathbf{a}_{1} + \mathbf{U}_{11}^{T} \, \mathbf{U}_{12} \, \mathbf{a}_{2} = \mathbf{U}_{11}^{T} \, \mathbf{d}, \tag{29a}$$

$$\mathbf{T}_{22}^T \, \mathbf{T}_{21} \, \mathbf{a}_1 + \mathbf{T}_{22}^T \, \mathbf{T}_{22} \, \mathbf{a}_2 = \mathbf{T}_{22}^T \, \mathbf{t}.$$
 (29b)

Expressing the LS-problem in this form we need not care for dimensioning in a and b parts of Eq. (28), respectively.

5. NUMERICAL EXAMPLES

The numerical experiments showed [18, 21] that the quadratic elements are good choice from the point of view both accuracy and algorithmic efficiency. The quadrilateral element which is similar as serendipity element in the displacement FEM formulation is defined by four boundary elements over the element. The definition of the element of arbitrary polygonal form is a simple task.

In the first example a square domain shown in Fig. 1 with prescribed load on its boundaries given by the 6-th order polynomial tractions was examined. In this way we could follow the errors in both displacement and stress fields in all points of the region. The tractions are chosen so that the lowest and largest gradients are in opposite corner points. The undeformed and deformed mesh of 10 x 10 elements (sub-domains) is shown in Fig. 1 and corresponding von Mises stress fields are given in Fig. 2. Figure 3 containes the mesh deformed by the vector of displacement errors in the nodal points (discrete values). We can see that the errors in displacements in the second case are much larger on the boundaries. The relative error of the extension of the diagonal (i.e. length between the corner nodes with smallest and largest gradients) is 2e-4 and similar value was obtained for maximal relative displacement error (related to the maximal displacement vector in the whole region — i.e. the displacement in the upper right corner node). The maximal relative error in the stress field (related to the maximal von Mises stress) was 2.5e-3. The smoothing procedure described in the Section 4 using the radius of the domain of influence equal to the length of the element diagonal and with the 3rd order Trefftz polynomials for the MLS interpolation was used and the errors are shown in Fig. 4. The maximal relative error of these values is 2e-4, which is one order better than that obtained by the simple averaging over the inter-element incompatibilities.

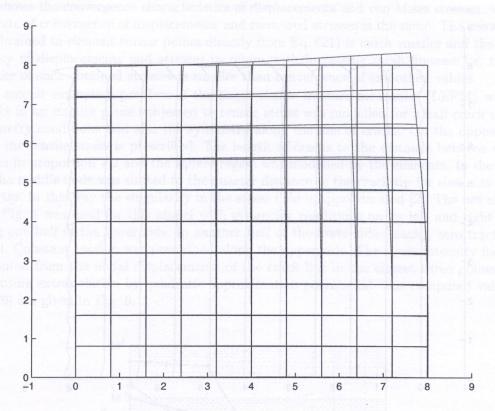


Fig. 1. Undeformed and deformed mesh

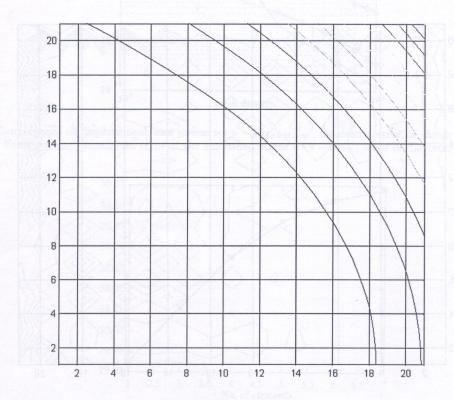


Fig. 2. Von Mises stress

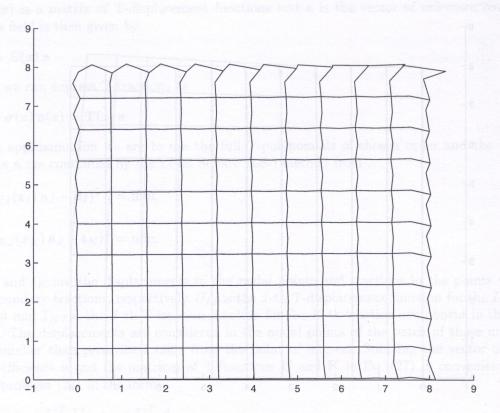


Fig. 3. Displacement errors

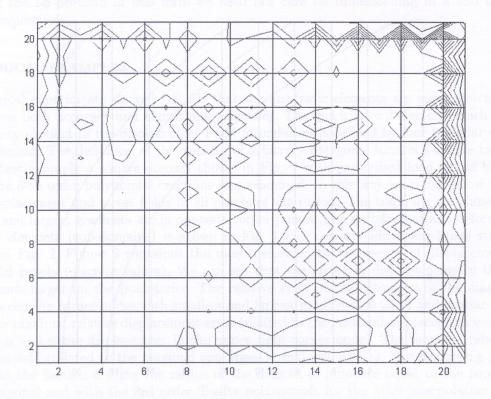


Fig. 4. Von Mises stress errors of the smoothed field

Figure 5 shows the convergence characteristics of displacements and von Mises stresses. We can see that the rate of convergence of displacements and recovered stresses is the same. The convergence of stresses obtained in element corner points directly from Eq. (21) is much smaller and the difference in accuracy of displacements and stresses increases with increasing mesh fineness i.e. the rate of convergence of such obtained stresses is smaller than convergence of smoothed values.

In the second example a problem of the linear elastic fracture mechanics (LEFM) was chosen. Line cracks in an infinite plane subjected to tensile stress was modelled for a half crack using both side symmetry conditions and also the symmetry along the line of cracks. On the opposite side of the crack the tensile stress is prescribed. The length of cracks to the distance between the cracks was chosen in proportion 1:2 and the square region was modelled by the elements. In the quadratic element the middle node was shifted to the quarter distance to the crack tip for elements modelling the crack tip. In this way the singularity in the stress field is approximated [2]. The net of elements shown in Fig. 1 was used for this model with symmetry conditions on its left and right sides and also along one half of the lower side. In another half of the lower side (crack), zero tractions were prescribed. Constant tension was prescribed along the upper side. The stress intensity factor (SIF) was computed from the nodal displacements of the crack line in the closest three points from the crack tip using extrapolation by quadratic approximation polynomial. The computed values of the SIF K_I [26] are given in Fig. 6.

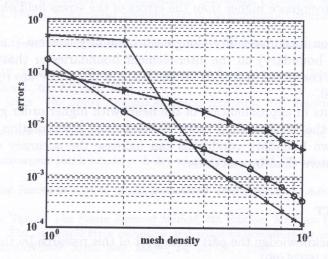


Fig. 5. Convergence of displacement and stress; $\triangleright \triangleright - \operatorname{Err}_{\sigma v M \operatorname{aver}}$, maximum error of the averaged stress, $\circ \circ \circ - \operatorname{Err}_{\sigma v M \operatorname{smooth}}$, maximum error of the smoothed stress * * * - Err_u , error of displacement norm

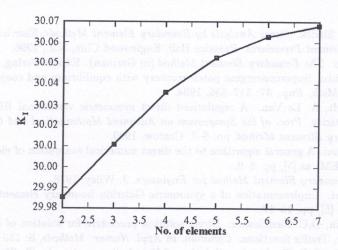


Fig. 6. Convergence of the stress and stress intensity factor K_I

6. CONCLUSIONS

In this paper a T-polynomial reciprocity based FEM is presented. The stiffness matrix for linear elasticity problems is computed by non-singular BIE. The T-polynomials can be obtained numerically or analytically by symbolic algebra also for higher order 3D polynomials as shown in the first part of this paper. The displacement are supposed to be compatible between the elements. The tractions are incompatible between the elements and the inter-element compatibility is satisfied in a weak sense by the variational formulation. The stiffness matrix defined in this way is symmetric and the elements can be arbitrarily combined with other displacement elements satisfying the condition of compatibility of displacements. The form of elements can be more general in our formulation, they can be even multiply connected. Also other (singular) formulations can be used in reciprocity relations and very large elements (multi-domain BEM with symmetric matrices resulting from the variational formulation for the inter-domain connectivity) can be formulated in this way. It is a simple problem to define transition elements joint to two or more elements along its one side.

The stresses obtained from the displacements in the nodal points using T-polynomial interpolation with MLS technique can give the stress field of the same accuracy as the primary computed displacements in the nodal points with the same rate of convergence. On the boundaries with prescribed tractions, inclusion of prescribed values into the local approximation improves the accuracy in these regions. The numerical examples show that the errors in stress fields are even one order or more lower and their convergence higher than the errors of the stress field obtained on the elements level.

Integral of the traction incompatibility along each boundary element (i.e. along the integration element on the element boundary) on the inter-element boundaries or that of the incompatibility between prescribed and computed tractions on the domain boundary are reliable error estimators for the local element [18].

Numerical experiments in approximation of the fields with higher order gradients show that the stress smoothing using the MLS method using T-polynomial interpolation from computed nodal displacements and known boundary conditions can increase the accuracy of the gradient (strain and stress) fields even more than by one order.

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