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POSTPROCESSING ERROR ESTIMATION TAKING TO THE ACCOUNT SINGULARITY EFFECT

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Abstract: - In this article the new method for the accounting singular point influence to the postprocessing error estimation is proposed. Solution improvement in singular zones is achieved modifying physical coordinate matrix used in least square problem equations: instead of the standard quadratic polynomial a new polynomial with singular elements is taken. Numerical examples demonstrate the advantages of the proposed algorithm.

Keywords: - Singular points, error estimation, least square method, adaptive mesh refinement.

1. Introduction

The evaluation of the discretization error and the design of suitable meshes via adaptive mesh refinement are nowadays two of the challenging issues in the finite element analysis. One of the main concerns in finite element analysis is the adequacy of the finite element mesh. Since the quality of the finite element approximated solutions directly depends on the quality of meshes, an additional process to improve the quality of meshes is necessary for reliable finite element approximations. In order to perform a reliable finite element simulation a number of researches have made efforts to develop an adaptive finite element analysis method which integrates the finite element analysis with error estimation and automatic mesh modification [1-3]. But sometimes even very effective adaptive mesh refinement strategy does not give us a suitable result if our problem domain is caused by re-entrant corners and abrupt changes in material properties. Singularities occur at crack tips and at interface problems and are of great interest from the point of view of failure analysis [4]. Singularities and unbounded domains cause difficulties in standard finite element analysis because they depend on the structure of eigen values and eigen functions in the vicinity of the singular points which may not be known a priori [5, 6]. For this reason a new method for solution improvement near singular points is presented in this paper. After incorporating this method into *h*-adaptive finite element analysis, a new strategy can be obtained, which takes less iteration number until the final optimal mesh is constructed. Proposed solution improvement algorithm is tested with numerical examples.

2. Basic concepts of error estimation

The point-wise discretization error is simply the difference between exact solution and the finite element solution:

$$e_u = u - u^h , \tag{1}$$

where $\boldsymbol{u}$ is the exact solution and $\boldsymbol{u}^h$ is the corresponding FE-approximation. In (1) the error has been referred to the prime variables of the finite element approximation (displacements). However, it can also be referred to the derivatives (stresses, the strains or other quantities of interest). The point-wise discretization error is difficult to interpret, so certain norms to measure error are used to assess finite element approximation. One of the most popular measurements of the discretization error is based on the energy norm, which originally was defined for elasticity problems, can be expressed as

$$\|e\| = \left(\int_\Omega e_u^T L e_u \, d\Omega \right)^{\frac{1}{2}} , \tag{2}$$

where $\boldsymbol{L}$ is differential operator of the governing equations.

The error norms over the whole domain Ω can be obtained as a summation from individual element Ω_k :

$$\|e\|^2 = \sum \|e\|_k^2 . \tag{3}$$

The absolute error defined by an energy norm is not convenient for use in practical computations. The dimensionless forms are favored and are customarily expressed as

$$\eta = \frac{\|e\|}{\|u\|} , \qquad \eta_k = \frac{\|e_k\|}{\|u\|} , \tag{4}$$

where $\|u\|$ is the strain energy norm, η and η_k are the relative global and relative element error, respectively.

Postprocessed error estimates are based upon information obtained during the solution process. The most important ingredient of the error estimation is the construction of the new solution of a higher quality since the exact solution for complex-engineering problems is generally unknown. Typically, this new improved solution is obtained by a posteriori procedure, which utilizes the original finite element solution itself. The essence of the postprocessed error estimator is to replace the exact solution with a postprocessed solution of higher quality:

$$\boldsymbol{e}_u \approx \bar{\boldsymbol{e}}_u = \boldsymbol{u}^* - \boldsymbol{u}^h , \qquad (5)$$

where $\bar{\boldsymbol{e}}_u$ is the point-wise estimated error. Using the improved solution we have an estimation of (2):

$$\|\bar{e}\| = \left(\int_{\Omega} \bar{e}_u^T L \bar{e}_u \, d\Omega \right)^{\frac{1}{2}} . \qquad (6)$$

In practice, we calculate this norm by summing over all elements in the domain Ω:

$$\|\bar{e}\|^2 = \sum_{i=1}^{nel} \|\bar{e}\|_i^2 = \sum_{i=1}^{nel} \int_{\Omega_i} \bar{\boldsymbol{e}}_u^T \boldsymbol{L} \bar{\boldsymbol{e}}_u \, d\Omega_i \ , \qquad (7)$$

where Ω_i is an element domain and *nel* is the total number of elements.

The most popular error estimation method is superconvergent patch recovery for displacements (SPRD) technique. The idea of the SPRD is to define a new displacement field of $p+1$ order over the patch elements [7]. This new field requires to be a least square fit to the original finite element solution at some points where the accuracy of finite element solution is higher. It has been known that the nodal points of the finite element approximation are found to be the exceptional points at which the prime variables (displacements) have higher order accuracy with respect to the global accuracy [8].

The new displacement field over the element mesh is calculated solving equation system for least square problem:

$$\left(\sum_j w_j^2 (Q(x_j))^T Q(x_j) \right) b_i = \left(\sum_j w_j^2 (Q(x_j))^T \right) (u_j^h)_i . \qquad (8)$$

There $Q = \begin{bmatrix} 1 & x & y & x^2 & xy & y^2 \end{bmatrix}$ is a row matrix containing monomial term of physical coordinates of $p+1$ order, and b is a set of unknown parameters to be determined. $w(x)$ is a positive weighting function with unity value for the element, defining the patch, and which decreases monotonically with increasing distance away from master element.

3. Postprocessing error estimation with singularity effect

3.1 Problem statement

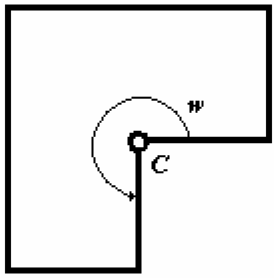

Fig.1 Problem domain

Let us suppose we have prismatic planar domain Ω with the interior angle $\omega > \pi$. C the singular point of Ω. Radius R is the value defining singular zone boundary for Ω (Fig.1).

In general solution u has singular behavior near singular points and can be decomposed into singular and regular parts according formula [9]:

$$u = u_s + u_R = \xi(r) \cdot \gamma(x) \cdot r^{\lambda} \cdot \sin \lambda\varphi + u_R , \qquad (9)$$

$$\lambda = \pi / \omega . \qquad (10)$$

There r, ϕ are polar coordinates, $\xi(r)$ is a smooth function ($\xi(r) = 1$ for $r < R$, $\xi(r) = 0$ for $r > R$, R is a constant), $\gamma(x)$ is a coefficient.

3.2 Displacement solution calculation near singularities

In order to use (9) formula in adaptive finite element analysis we must find regular and singular parts of the solution u.

As a regular part we can take finite element solution $u_R = u_{FEM}$. For finding singular part, we will modify SPRD method as follows.

Let us suppose domain Ω is covered by N triangle elements:

$$T = \{ T_i | i = 1, \Lambda \ , N \} . \qquad (11)$$

Current mesh element is said to be singular if at least one its nodes is placed at the distance less or equal to radius R. Set of all singular triangles defines singular zone of Ω and forms the patch for the least square problem:

$$\Omega_{SING} = \left\{ T_i \middle| \| Node_j (T_i) \| \le R_0 \, j = 1,2,3 \right\} . \qquad (12)$$

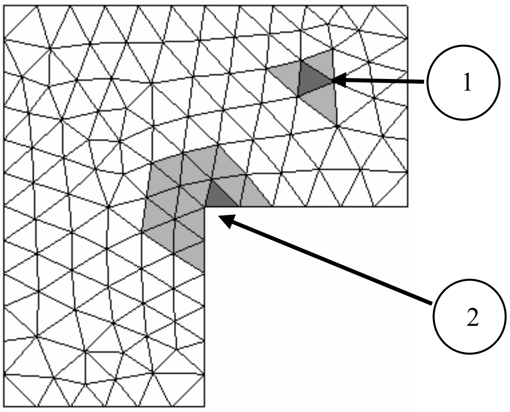

Fig.2 Element patch construction for least square problem: (1) – traditional element patch; (2) – singular element patch.

The main idea of least square method modification is to replace row matrix containing monomial term of physical coordinates with new one containing singular monomials for all nodes of this singular patch. To realize this instead of standard quadratic polynomial we will take only one singular monomial:

$$Q(x) \to Q_{SING}(r,\phi) = \left[\xi(r) \cdot r^{\lambda} \cdot \sin \lambda\phi\right]. \qquad (13)$$

According such modification equation system for least square problem will be solved with two different element patch types (Fig.2) and row matrixes depending on whether node $Node_j(T_i)$ belongs to singularity zone or no:

$$Q = \begin{cases} Q(x), & dist(C, Node_j(T_i)) \geq R_0, \\ Q_{SING}(r,\varphi), & dist(C, Node_j(T_i)) < R_0. \end{cases} \qquad (14)$$

But in this place we have one problem left: singular point C in polar coordinates is defined as $r=0$ and $\phi \in [0,2\pi]$ and singular polynomial can not be defined correctly in point *C!*

In order to solve this conflict, additional points placed at a very near position from C must be constructed. For all mesh elements containing singular point C we calculate additional points C_i placed at a very near position from original point C (Fig.3):

$$C_i = (1-t) \cdot C + t \cdot D_i, \qquad (15)$$

$$D_i = \frac{1}{2} \cdot \left(\frac{1}{2} \cdot A_i + \frac{1}{2} \cdot C\right) + \frac{1}{2} \cdot \left(\frac{1}{2} \cdot B_i + \frac{1}{2} \cdot C\right), \qquad (16)$$

$$t = \frac{t}{\sqrt{N}} \cdot \frac{const}{\|CD_i\|}. \qquad (17)$$

In these equations A_i and B_i are the nodes of singular element, D_i – point on bisector from point C, N – number of mesh elements, h – the size of smallest mesh element, $\|CD_i\|$ – the distance from point C to point D_i, $const \in (0,1]$ – the smoothing value. The definition of parameter t allows us to control positions of new C_i: the ratio $h/\sqrt{N}$ guarantees that new point C_i will be bounded by sides of singular element, and division by $\|CD_i\|$ guarantees that C_i will be placed near original point.

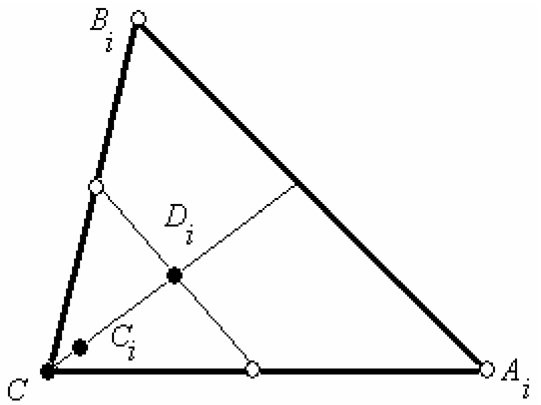

Fig.3 Definition of additional points near singularity

For all nodes from the singular patch Ω_{SING} we form physical coordinate vector:

$$x_{SING}(x_k, y_k) = x_{SING}(r_k \cdot \cos\phi_k, r_k \cdot \sin\phi_k) \qquad (18)$$

and define singular polynomial:

$$Q_s(r,\phi) = \left[\xi(r) r^{\lambda} \sin \lambda\varphi\right]. \qquad (19)$$

After transformation displacement vector to polar coordinates we obtain following equation system:

$$\left(\sum_i w_j^2 \left(Q_{SING}(x_{SING,j})\right)^T Q_{SING}(x_{SING,j})\right) b_{SING,j} =$$

$$= \left(\sum_i w_j^2 \left(Q_{SING}(x_{SING,j})\right)^T\right) \left(u_{SING,j}^h\right)_i. \qquad (20)$$

After solving least square method equations with singular patch and singular polynomial we get coefficient vector b_{SING} and for each additional singular point C_i we calculate singular displacement solution:

$$u(C_j) = u_{FEM}(C_j) + u_S(C_j) =$$

$$= u_{FEM}(C_j) + Q_{SING}(C_j) \cdot b_{SING}(C_j). \qquad (21)$$

General solution for singular point C is obtained using extrapolation from additional singular displacement solutions in points C_i.

3.3 Error estimation near singularities

After the improved solution in point C is calculated, it can be taken instead of the exact solution in the posteriori error estimation:

$$\boldsymbol{e}_{u,SING} \approx \bar{\boldsymbol{e}}_{u,SING} = \boldsymbol{u}^*_{SING} - \boldsymbol{u}^h , \quad (22)$$

there $\bar{\boldsymbol{e}}_{u,SING}$ is the point-wise estimated error for singular zone of the problem domain.

An estimation of the whole domain errors can be calculated summing error values from the singular zone and the rest part of the problem domain:

$$\|\bar{e}\|^2 = \|\bar{e}\|^2_{\Omega_{SING}} + \|\bar{e}\|^2_{\Omega\text{-}\Omega_{SING}} , \quad (23)$$

there $\|\bar{e}\|^2_{\Omega_{SING}}$ – estimated error for singular zone only and $\|\bar{e}\|^2_{\Omega\text{-}\Omega_{SING}}$ – estimated error for the rest part of the problem domain.

4. Numerical example

For demonstration of the proposed solution improvement algorithm L-Shape domain (Fig.4) is considered. Plane stress conditions are assumed with Poison's ratio ν=0.3 and Young's modulus E=10^5 Pa. Permissible error tolerance is η=5%.

The goal is to obtain final optimal mesh with as small element number as possible according given permissible error. In order to achieve this goal we should improve solution in the first adaptive mesh refinement strategy steps when total element number is quite small, because after few iterations element number is increased rapidly and obtained solution does not differ from the exact solution very much. For this reason we will generate a set of meshes with gradually increasing element number and will analyze improved postprocessed solution efficiency in comparison with not improved postprocessed solution.

In order to test proposed strategy we construct a set of uniform unstructured meshes where element number is increased according given formula:

$$N_i \approx \begin{cases} N_0 + i*200, & if \quad i \le 8, \\ 2*N_{i-1}, & if \quad 8 < i \le 10, \\ 9500, & if \quad i = 11, \\ 16222, & if \quad i = 12. \end{cases} \quad (24)$$

There $N_0 = 206$ is the element number of the first mesh, i=1,…,12 is the mesh index.

Periodically increasing element number (from 206 elements to 16222 elements) twelve different finite element meshes are generated. Singular zone is defined by radius $R = 0.1$ and singular element patch is combined from all elements having at least one node placed at the distance less or equal to radius $R = 0.1$. First three meshes (with 206, 418 and 600 elements respectively) from this set and their singular zones are showed in Fig.5, Fig.6 and Fig.7. Obtained singular zone region is marked in grey color and zoomed in for better viewing. For

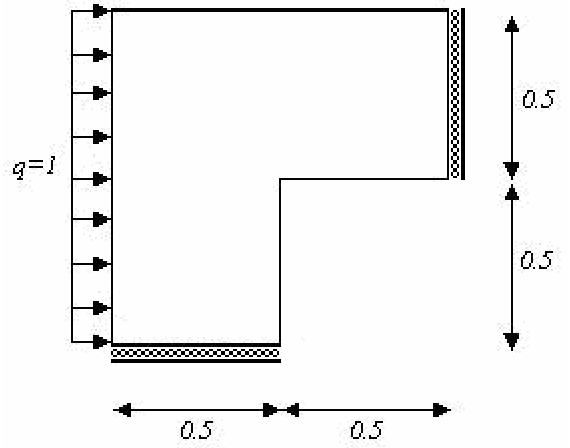

Fig. 4 L-shape domain definition

each mesh the finite element analysis is performed and finite element solution is calculated. After that postprocessing error estimation is performed in two cases: the first experiment is to calculate postprocessing solution without special improvement in singular zone and the second experiment is performed improving postprocessing solution in singular zone according proposed strategy.

Graphical presentation of the obtained displacement results in Ux and Uy directions is presented in Fig.8. Exact displacement solution for such L-shape problem is not known and for comparing results additional mesh with 25000 elements is generated and obtained displacement solution is taken instead of the exact.

Comparing obtained results we can see that already for mesh with 1004 elements improved singular postprocessing displacement solution in X direction (Fig.8) is almost equal to the exact solution and is not changing very much when element number in the mesh is increased:

$UX_{SING,1004} = 2.3585e^{-4}$, $UX_{EX} = 2.362e^{-4}$,

$UX_{EX} - UX_{SING,1004} = 0.0415e^{-4} \approx 0.0;$

$UX_{EX} - UX_{SING,16222} = 0.0417e^{-4} \approx 0.0.$

Situation with improved singular postprocessing displacement solution in Y direction (Fig.8) is very similar – obtained improved solution is much more near the exact solution than postprocessing solution without improvement in singularity zone:

$UY_{SING,1004} = 1.4621e^{-4}$, $UY_{1004} = 1.4388e^{-4}$,

$UX_{EX} - UX_{SING,1004} = 0.04887e^{-4}$,

$UX_{EX} - UX_{1004} = 0.0722e^{-4}$.

According these graphical displacement curves, we can see that improved singular postprocessing solution is calculated more exactly than finite element solution and converges to the exact solution sooner than finite element solution

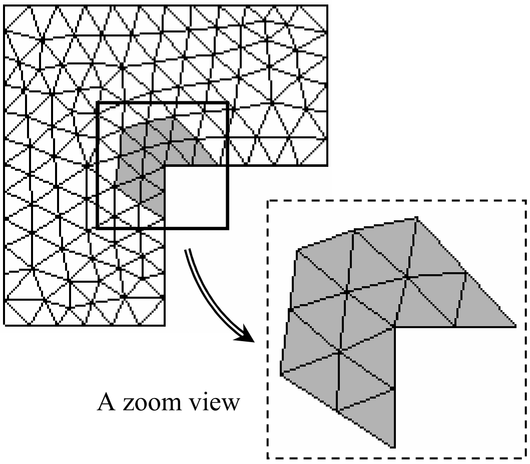

Fig.5 Singular patch for 206 element mesh

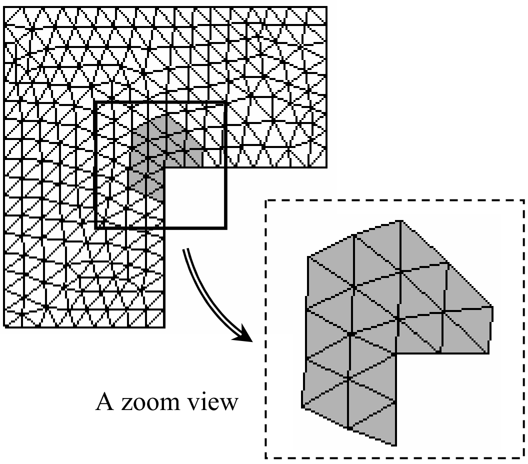

Fig.6 Singular patch for 418 element mesh

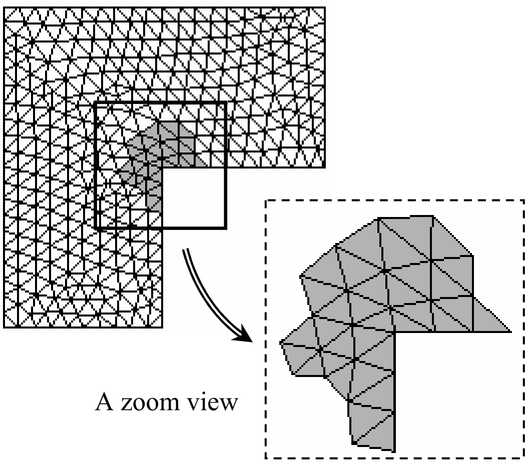

Fig.7 Singular patch for 600 element mesh

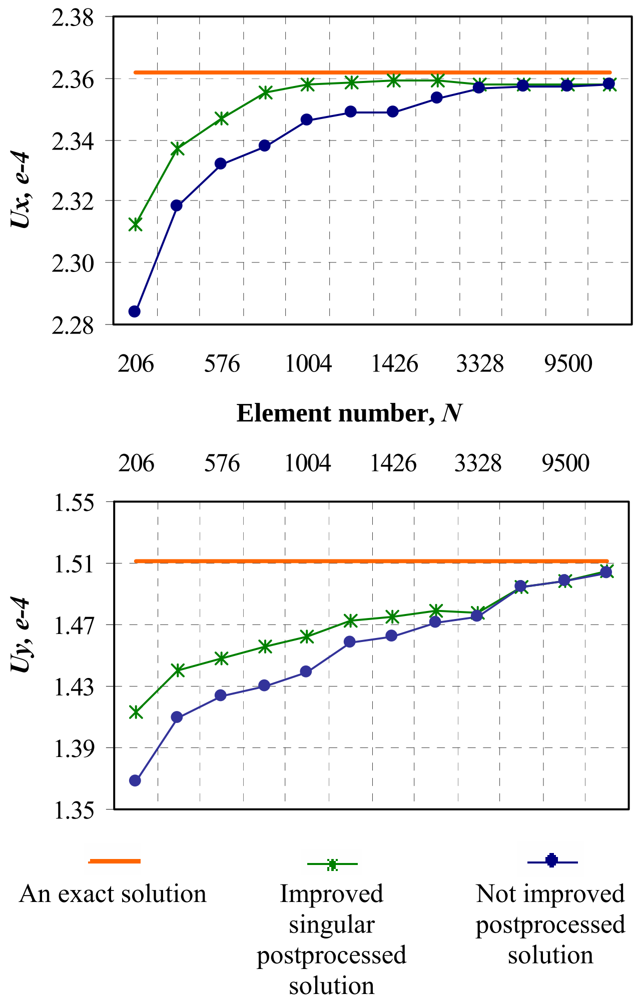

Fig.8 Displacement curves in *Ux* and *Uy* direction

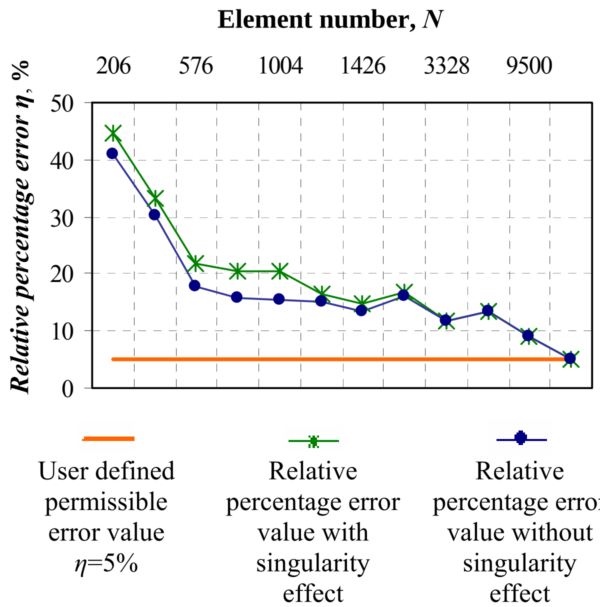

Fig.9 Comparison of the obtained relative percentage error values

To demonstrate more clearly the advantage of the proposed solution improvement strategy near singularities an additional comparison of the estimated relative errors presented in Fig.9. The curves in this picture are calculated using error data only from singular domain (grey color) because summing error values from the whole domain the impact of improved solution vanishes and is not so obvious. Comparing obtained relative percentage error values we can see that the difference between user defined value and value calculated according proposed solution improvement near singular point is bigger than difference, obtained between user defined value and value, calculated according traditional error estimation algorithm. It means that displacement solution was really improved in singular point zone and obtained error value is calculated more precisely than error value without singularity improvement.

It is proved by authors [10] that incorporating this solution improvement strategy into standard *h*-adaptive finite element strategy final optimal mesh is obtained with least iteration number and least total element number in comparison with traditional adaptive mesh refinement algorithm.

5. Conclusions

In this paper a new method for postprocessed solution improvement near singularities is presented and tested. In order to involve the influence of singular domain zones displacement solution was calculated with modified least square method. Summarizing can be stated that taking singular polynomial instead of the standard quadratic in the postprocessed solution calculation we can define solution more precisely in domains with different topological incompatibilities. It can also be expected that after incorporating proposed changes to the standard adaptive mesh refinement procedure we will get final optimal mesh with the least iteration number and with minimal element number in it.

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