THE COMPUTATIONAL MODELS FOR SIMULATION OF CAVITY MICROSTRUCTURE

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Abstract: The paper deals with the 2D and 3D computational problems for simulation of cavity microstructure. The cavities, holes and other in-homogeneities cased the stress concentration in material microstructure. The aim is to develop the effective computational models which best simulate both near and far fields. The Method of External Finite Element Approximation (MEFEA) is applied to simulate detailed stress state. The results are compared with both analytical solution (if it exists) and p-version of classical FEM (pFEM).

Key words: cavity, stress concentration, T-elements, p-elements, comparison

1 INTRODUCTION

Accurate enough computation of stress field is required in order to evaluate static and dynamic (fatigue) behaviour and bearing capacity of the structure. Holes and different cavities are frequent structural concentrators. Computations, especially in 3D, and moreover in problems containing the interaction with other types of stress concentrators (cracks, stiff or weak inclusions, inhomogenities, etc.), require large computational times and are also cumbersome for preparation of models, especially if volume elements (FEM, FVM) are used for the modelling. Meshless methods working with volume approximation are simpler, but need even more equations than FEM and FVM to achieve similar accuracy.

In this paper, a Method of External Finite Element Approximation (MEFEA) will be presented to model stress concentration problems. MEFEA is an enhanced classic FEM with idea of external approximations. The method does not need discretization by classical elements, however, instead of elements the domain is divided into Trefftz type subdomains. There are shape functions in the discrete solution space that do not belong to the infinite dimensional solution space. The domain is split in subdomains (cells) and the approximation is built on each of these subdomains independently of each other.

2 MEFEA AND DEGREES OF FREEDOM

The method is similar to Hybrid Trefftz Finite Element Method, where Trefftz functions are used inside of each element (subdomain). The displacement and force boundary conditions are met only approximately whereas the governing equations are fulfilled exactly in the volume for linear elasticity, making it possible to assess accuracy in terms of error in boundary conditions. The main benefit is that the discretization can be done directly on a 3D CAD geometry with all details (features) for the analysis.
In MEF A the degrees of freedom have no physical meaning comparing with traditional FEM where degrees of freedom are displacement of nodes, temperature, etc. There are three types of degrees of freedom: Boundary DOF, Internal DOF and Concentrator DOF. Concentrator DOFs are functions associated with the surfaces which cause stress concentration. They correspond to the special basic functions intended to accurately simulate the stress state near stress concentration regions.

The special basic functions are \( f_i = \frac{1}{r} \), a concentrator basis function with asymptotic behaviour (radial functions), \( i=1, 2, \ldots, n \) is the number of concentrator degrees of freedom.

\[
\mathbf{u} = \sum_{i=1}^{n} N_i \mathbf{c}_i + \sum_{i=1}^{m} f_i \mathbf{a}_i
\]

(1)

Functions \( N_i \) approximate the global behaviour of the structure. Functions \( f_i \) approximate the local behaviour around the holes, different cavities, cracks, stiff or weak inclusions, inhomogenities and other structural concentrators.

3 2D AND 3D PROBLEMS WITH STRESS CONCENTRATION

In the following, 2D and 3D problems with stress concentration using the Trefftz functions are presented. The modeled stress concentrators are holes and cavities of spherical and ellipsoidal shapes. Moreover, the random spherical cavity microstructure is modelled. The Method of External Finite Element Approximation (MEFEA) is applied to simulate detailed stress state of mentioned stress concentrators. The results are compared with both analytical solution (if it exists) and p-version of classical FEM (pFEM). With p-version of FEM, local areas of stress concentration are simulated with elements with high polynomial order. To refine the approximate solution, the element size is kept constant and element p-order is increased.

3.1 Finite-width plate with a circular cavity

The 2D problem is modelled for central circular cavity (hole) (Fig. 1) \( a = 1\text{mm}, \ b = 5\text{mm}, \ E = 1\text{MPa}, \ \nu = 0.3 \) and \( p = 1\text{MPa}. \) The analytical solution for the stress \( \sigma_{rr} \) and \( \sigma_{\theta\theta} \) in plane \( y = 0 \) is given by [3]:

\[
\sigma_{rr} = \frac{p}{2} \left[ \left( 1 - \frac{a^2}{r^2} \right) - \left( 1 - \frac{4a^2}{r^2} + \frac{3a^4}{r^4} \right) \right] ; \quad \sigma_{\theta\theta} = \frac{p}{2} \left[ \left( 1 + \frac{a^2}{r^2} \right) - \left( 1 + \frac{3a^4}{r^4} \right) \right]
\]

(2)

Fig. 1 One quarter of finite-width plate with a circular cavity and split
The domain is meshed with 293 p-elements (tetrahedrons) with maximum order 5 and the domain is split with 4 subparts (Fig. 1) with order 5.

![Tangential Stress Graph](image)

**Fig. 2** *Comparison of tangential stresses $\sigma_{\theta\theta}$ along x-axis*

### 3.2 3D Kirsch problem

The 3D problem illustrates the state of stress in the vicinity of a cavity by uniaxial stress in infinity (Fig. 3). The problem is modelled for $a = 1\text{mm}$, $b = 10\text{mm}$, $p = 1\text{MPa}$ and $\nu = 0.27$. The analytical solution for normal stress $\sigma_{yy}$ in plane $y = 0$ is given as [3]:

$$
\sigma_{yy} = p \left[ 1 + \frac{4 - 5\nu}{2(7 - 5\nu)} \left( \frac{a}{r} \right)^3 + \frac{9}{2(7 - 5\nu)} \left( \frac{a}{r} \right)^5 \right]
$$

where $r$ is the radial distance from centre of the cube to the point of interest.

![3D Kirsch problem and split](image)

**Fig. 3** *3D Kirsch problem and split*

Figure 3 shows the comparison among the analytical solution and numerical solutions presented by pFEM and MEFEA. The domain is meshed with 1301 p-elements (tetrahedrons) with maximum order 4 and the domain is split with 28 subdomains (Fig. 3) with order 4.
Stress concentrators are added to the solution on the inner surface of cavity.

![Stress σyy along x-axis](image)

**Fig. 4** Comparison of $\sigma_{yy}$ along the x-axis for Kirsch problem

### 3.3 Modified 3D Lame problem with ellipsoidal cavity

The problem is modelled for sphere of radius $r = 1$mm with central ellipsoidal cavity (Fig. 5).

![Modified 3D Lame problem with ellipsoidal cavity and quarter of model and detail of split](image)

**Fig. 5** Modified 3D Lame problem with ellipsoidal cavity and quarter of model and detail of split

The cavity is represented as an ellipsoid with the long (semi-major) axis $a = 1$ mm and semi-minor axis $b = 0.2$mm, $E = 1$MPa, $\nu = 0.3$ and internal pressure $p = 1$MPa. The length of the ellipse is $2a$ and its width is $2b$ (Fig. 5).

The dashed line shows the part of model where detail of split is depicted.

Figure 6 shows the comparison between numerical solutions presented by MEFEA and pFEM. The domain is meshed with 267 p-elements (tetrahedrons) with maximum order 5. The MEFEA model consist of 79 subdomains with orders 4, 5 a 6. Stress concentrators are added to the solution. The results are the same. The match between results is very good.
3.4 3D random spherical cavity microstructure

3D random spherical cavity microstructure is representative of more complex structure (Fig. 7). The discontinuities are spherical cavities with diameter $d = 0.4\text{mm}$. The control volume of microstructure consists of 16 randomly situated cavities of the same size. The size of control volume is $b = 2\text{mm}$. The upper surface has prescribed displacement $u_y = 5\times10^{-5}\text{mm}$. The symmetry conditions are applied for all other surfaces of control volume. Modulus of elasticity $E = 2\times10^5\text{MPa}$ and $\nu = 0.27$. Whereas the analytical solution does not exist for such problem, the comparison results are results computed by pFEM.

Figure 15 shows the comparison between numerical solutions presented by MEFEA and pFEM. The domain is meshed with 1963 p-elements (tetrahedrons) with maximum order 7. The MEFEA model consist of only 1 subpart with order 4. Stress concentrators are added to the solution.
The cavity marked by X (Fig. 7) is the cavity of the maximum Stress YY detected both MEF EA (12.0 MPa) and pFEM (12.8 MPa).

4 CONCLUSIONS

The computational simulation is source of design ideas and applications, and will provide a good understanding of how microstructure affects the properties of materials.

The typical procedure in science is to begin from the real material, predict the material behaviour, and then compare with experiment. But theory can also be used in an inverse way. We can begin with a theoretical concept of an interesting property or effect, formulate a hypothetical structure via computational simulation then make the laboratory testing and actually make the material. The inverse procedure is very interesting for theory, and for materials science, as it can lead to entirely new materials.

In this paper, the computational simulation of holes and different cavities of spherical and ellipsoidal shapes as frequent structural concentrators was performed using classical displacement FEM formulation using p-refinement and a Trefftz-type FEM formulation called the Method of External Finite Element Approximation (MEFEA). The use of large T-elements make possible to reduce the problem also reduces the number of subdomains. However, the special stress concentration functions and mentioned large T-elements are used; the higher density of subdomains is needed to appropriately simulate stress state.

We will continue in this research and the present results will be used for further development of simulation materials with microstructure.

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6 REFERENCES


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