Programming an XFEM routine to investigate the effect of Hole(s) and inclusion(s) in a plate (2D)

Personal Programming Project (2022-2023)

Nandha Gopal Mariappan

Date of the Defence Presentation : 14/06/2023
Matriculation Number : 66994

Project Supervised by : Dr.-Ing. Stefan Prüger

Incharge for Personal Programming Project :

Dr. Arun Prakash and Dr.-Ing. Stefan Prüger

1.Introduction/Motivation:-

- Finite Element Method (FEM) is one of the greatest numerical tool for the simulation of discontinuities and fracture problems.
- During the meshing process of materials with multiple discontinuities (cracks, holes and inclusions),the modelling and simulation using FEM becomes quite cumbersome.
- To overcome these difficulties, Belytschko and Black(1999) proposed a new computational method called the "extended finite element method (XFEM)".
- One of the best Numerical technique XFEM allows the modeling of the heterogeneities(Holes, inclusions and cracks) independent of the mesh and provides the accurate result.
- The highlight of the XFEM : To help tackle problems with localized features that are inefficiently resolved by mesh refinement.
- The XFEM approximation consists :
  1. Standard finite elements used throughout the domain.
  2. Enriched elements used in the enriched sub-domain to capture specific solution features such as discontinuities and singularities.
- In this project, I have implemented a XFEM routine to investigate the effect of hole(s) and inclusion(s) in a plate (2D).

2.Task and aims of the project:-

- The main aim of this project is to find the stress contours and displacement contours of the plate having hole(s) or inclusion(s) in both x and y direction by applying the XFEM numerical technique.

- For that, a plate having linearly elastic isotropic material behaviour having hole(s) or inclusion(s) or both is subjected to uniaxial tension under different load conditions with appropriate Dirichlet Boundary conditions applied to the edges/cornernodes of the plate.

- For the first case of the validation of the program, one example was taken from book (Khoei, A. R. (2014). *Extended finite element method: theory and applications*. John Wiley & Sons.) where the stress contours of x and y direction will be compared with the stress contours generated from this project.

- For the second case of the validation of the program, a journal paper(Jiang, S., Du, C., & Gu, C. (2014). An investigation into the effects of voids, inclusions and minor cracks on major crack propagation by using XFEM. *Structural Engineering and Mechanics*, *49*(5), 597-618.) results have been compared, where the displacement contours of x and y direction will be compared with the displacement contours generated from this project.

- Programming Language Used : Python 3.10.8

- Libraries Used : math, Numpy, Sympy, matplotlib, pathlib are the total list of libraries used in the program.

3.Theory of the implemented project:-

3.1Strong form to weak form:-

- Strong form equation : $\nabla.\sigma + b = 0$ where $\sigma = C : \varepsilon$ and $\varepsilon = \nabla_s u$ [1]

where ∇u is the symmetric gradient operator, C is the tensor of elastic moduli for a homogenous isotropic material and b is the body force vector.

- By applying associated boundary conditions, the strong form of the equation can be written as (given below)

$$\int_{\Omega} \boldsymbol{\sigma}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{v})\, d\Omega = \int_{\Omega} \mathbf{b} \cdot \mathbf{v}\, d\Omega + \int_{\Gamma_t} \bar{\mathbf{t}} \cdot \mathbf{v}\, d\Gamma \quad [2]$$

- By substituting the trial and test functions in weak form equation, it will be converted to discrete equation which is $[K]\{d\}$ =$\{\mathrm{f}\}$ where K is the Global stiffness Tensor, d is the vector of unknown nodal displacements and f is the external force vector.

3.2Shape functions and Gauss quadrature points:-

- Gauss Integration of a quadrilateral element is given by equation(3) taken from *Fish, J., & Belytschko, T. (2007). A first course in finite elements (Vol. 1). New York: Wiley.*

$$\mathbf{I} = \sum_{i=1}^{2} \sum_{j=1}^{2} \mathrm{W}_i \mathrm{W}_j |\mathbf{J}^e(\xi,\eta)| \mathrm{f}(\xi,\eta)\, d\xi\, d\eta \quad [3]$$

$$\mathbf{N_1}(\xi,\eta) = \frac{1}{4}(1-\xi)(1-\eta)$$
$$\mathbf{N_2}(\xi,\eta) = \frac{1}{4}(1+\xi)(1-\eta) \quad [4]$$
$$\mathbf{N_3}(\xi,\eta) = \frac{1}{4}(1+\xi)(1+\eta)$$
$$\mathbf{N_4}(\xi,\eta) = \frac{1}{4}(1-\xi)(1+\eta)$$

- Shape functions taken from *(fish and Belytschko 2007)* used in this project

Points	ξ	η	Weights(W_i and W_j)
1	$-\frac{1}{\sqrt{3}}$	$-\frac{1}{\sqrt{3}}$	1
2	$-\frac{1}{\sqrt{3}}$	$\frac{1}{\sqrt{3}}$	1
3	$\frac{1}{\sqrt{3}}$	$-\frac{1}{\sqrt{3}}$	1
4	$\frac{1}{\sqrt{3}}$	$\frac{1}{\sqrt{3}}$	1

Table1 : Coordinates and weights of 2x2 Gauss quadrature *(fish and Belytschko 2007)*

3.3 Node numbering and element numbering :-

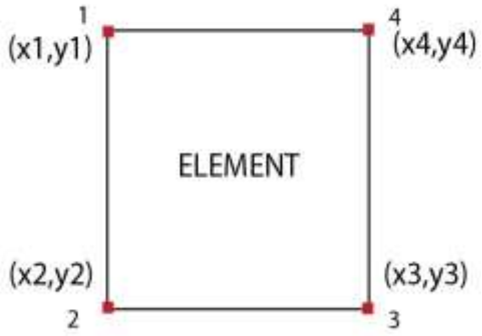


Figure1 : Node numbering of an element

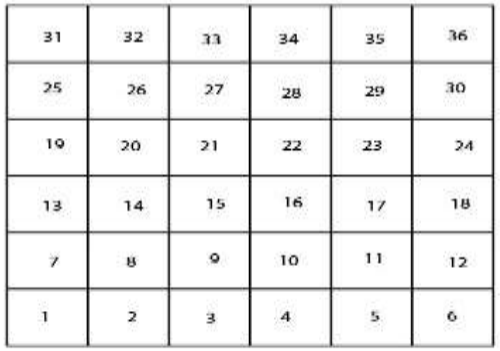


Figure2 : Element numbering in a plate

- Node numbering and edge numbering carried out in this project

3.4 Level set method :-

- Different techniques can be employed for enrichment function depends on type of discontinuity.
- Signed distance function, Heaviside function, Level set function and branch function – Among these Level set function is used in this project.
- **Reasons** : Better for Weak discontinuities like Holes and inclusions.
  Provide accurate solutions for different material properties used in the model

$$\varphi = \sqrt{x - x_1 + y - y_1} + \mathrm{r} \quad [5]$$

Level set function equation(5) taken from [Sukumar, N., Chopp, D. L., Moës, N., & Belytschko, T. (2001). Modeling holes and inclusions by level sets in the extended finite-element method. Computer methods in applied mechanics and engineering, 190(46-47), 6183-6200.]

- $\varphi > 0$ → outside the discontinuity, $\varphi = 0$ → on the boundary of discontinuity, $\varphi < 0$ → inside the discontinuity.

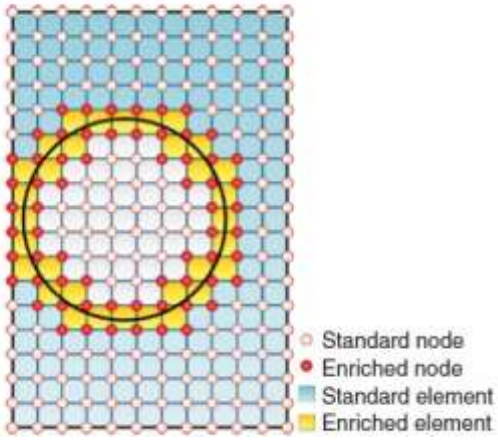


Figure3:Differentiating standard and enriched elements in a plate [(Khoei,2014)]

3.5 Rectangular sub-grids method :-

- Triangular/quadrilateral partitioning method and rectangular sub-grid method are two methods - used for numerical integrations of enriched element.
- In this project, rectangular sub-grid method (3*3) = 9 sub grids is implemented.(Ref : Figure4)
- **Reasons** : It is easy to implement than the other
  Adequate accuracy – increasing the number of grids

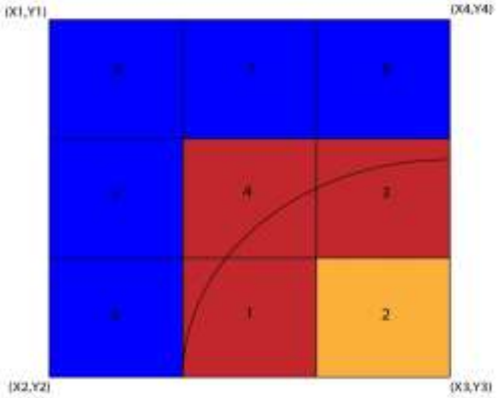


Figure4: Rectangular sub-grid method used in an enriched element

3.6 B-matrix for standard and enriched elements:-

$$\mathbf{B}^{std}_{3\times 8} = \begin{bmatrix} N_{1,x} & 0 & N_{2,x} & 0 & N_{3,x} & 0 & N_{4,x} & 0 \\ 0 & N_{1,y} & 0 & N_{2,y} & 0 & N_{3,y} & 0 & N_{4,y} \\ N_{1,y} & N_{1,x} & N_{2,y} & N_{2,x} & N_{3,y} & N_{3,x} & N_{4,y} & N_{4,x} \end{bmatrix} \quad [6]$$

B-matrix for standard elements (Khoei,2014)

$$\mathbf{B}^{enh}_{3\times 16} = \begin{bmatrix} N_{1,x} & 0 & (N_1\bar{\psi}_1)_{,x} & 0 & \cdots & N_{4,x} & 0 & (N_{4,x}\bar{\psi}_4)_{,x} & 0 \\ 0 & N_{1,y} & 0 & (N_1\bar{\psi}_1)_{,y} & \cdots & 0 & N_{4,y} & 0 & (N_4\bar{\psi}_4)_{,y} \\ N_{1,y} & N_{1,x} & (N_1\bar{\psi}_1)_{,y} & (N_1\bar{\psi}_1)_{,x} & \cdots & N_{4,y} & N_{4,x} & (N_4\bar{\psi}_4)_{,y} & (N_4\bar{\psi}_4)_{,x} \end{bmatrix} \quad [7]$$

B-matrix for enhanced elements (Khoei,2014)

3.7 Stress/Strain or Constitutive [D} matrix and Jacobi Matrix :-

$$\mathbf{D}_{3\times 3} = \frac{\mathrm{E}}{1-\nu^2}\begin{bmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & \frac{1-\nu}{2} \end{bmatrix} \quad [8]$$

Plane stress condition

$$\mathbf{D}_{3\times 3} = \frac{\mathrm{E}}{(1+\nu)(1-2\nu)}\begin{bmatrix} 1-\nu & \nu & 0 \\ \nu & 1-\nu & 0 \\ 0 & 0 & \frac{1-2\nu}{2} \end{bmatrix} \quad [9]$$

Plane strain condition

$$\mathbf{J} = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} \end{bmatrix} = \begin{bmatrix} \sum_{I=1}^{4} \frac{\partial \mathrm{N_I}}{\partial \xi}\mathrm{x}_I & \sum_{I=1}^{4} \frac{\partial \mathrm{N_I}}{\partial \xi}\mathrm{y}_I \\ \sum_{I=1}^{4} \frac{\partial \mathrm{N_I}}{\partial \eta}\mathrm{x}_I & \sum_{I=1}^{4} \frac{\partial \mathrm{N_I}}{\partial \eta}\mathrm{y}_I \end{bmatrix} \quad [10]$$

Jacobi matrix (Khoei,2014)

3.8 Stiffness matrix :-

- Stiffness matrix for standard element. (Khoei,2014)

$$K_{8\times8}^{std} = \sum_{i=1}^{2}\sum_{j=2}^{2} W_i W_j B^{e^T}(\xi_i,\eta_j)\, D^e\, B^e(\xi_i,\eta_j)\,|J^e(\xi_i,\eta_j)| \qquad [11]$$

- Stiffness matrix for enhanced element(both standard and enriched part)

$$K_{16\times16}^{enh} = \sum_{k=1}^{9}\sum_{i=1}^{2}\sum_{j=2}^{2} W_i W_j B^{e^T}(\xi_i,\eta_j)\, D^e\, B^e(\xi_i,\eta_j)\,|J^{sub}(\xi_i,\eta_j)|\,|J^e(\xi_i,\eta_j)| \qquad [12]$$

3.9 Body force and Traction force:-

- The body force of an element is calculated using the below equation *(fish and Belytschko 2007)*

$$\mathbf{f_{b}}_{8\times1} = \int_{-1}^{1}\int_{-1}^{1} [\mathrm{N}]^{\mathbf{T}}\, \mathbf{b}\, \mathbf{t}\, |\mathbf{J}|\, d\boldsymbol{\xi}\, d\boldsymbol{\eta} \qquad [13]$$

- The traction force of the edge of the element is calculated using the below equation *(fish and Belytschko 2007)*

$$\mathbf{f_{s}}_{4\times1} = \int_{-1}^{1} [\mathrm{N}]^{\mathbf{T}}\, \mathbf{T}\, \mathbf{t}\, |\mathbf{J}|\, d\boldsymbol{\xi} \qquad [14]$$

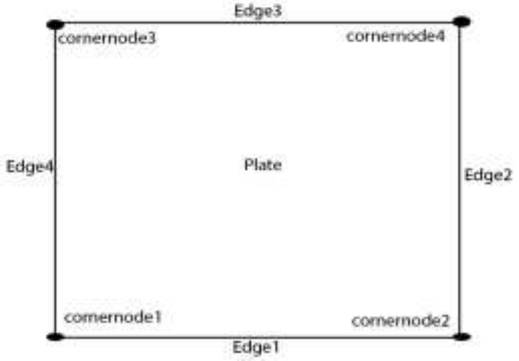


Figure5:Edge numbering and corner node numbering for applying traction force and Dirichlet Boundary conditions

3.10 Solving Linear system of equations:-

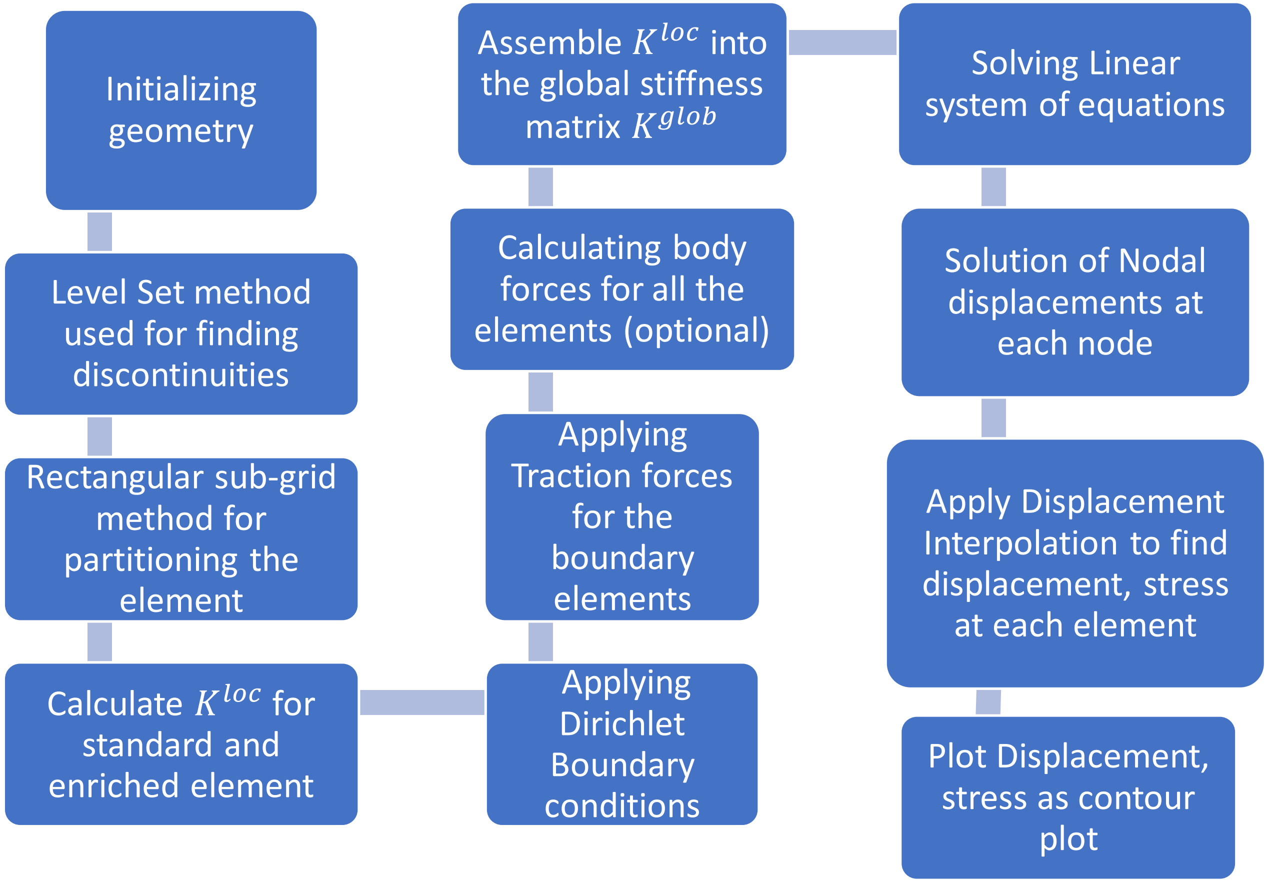
- After applying Dirichlet Boundary conditions, solve the linear system of equations $[K]\{u\} = \{F\}$ and find the nodal displacements.

3.11 Extraction of results:-

- By using Displacement interpolation to find the displacement at the element centroid (Bhatti, M. A. (2005). Fundamental finite element analysis and applications: with Mathematica and Matlab computations. Stress and Strains have also been found.

Displacements = $N^T d$ [15] **Strain**(ϵ) = $B^T d$ [16] **Stress**(σ) $=$ D ϵ [17]

4.Flowchart of the implemented code:-

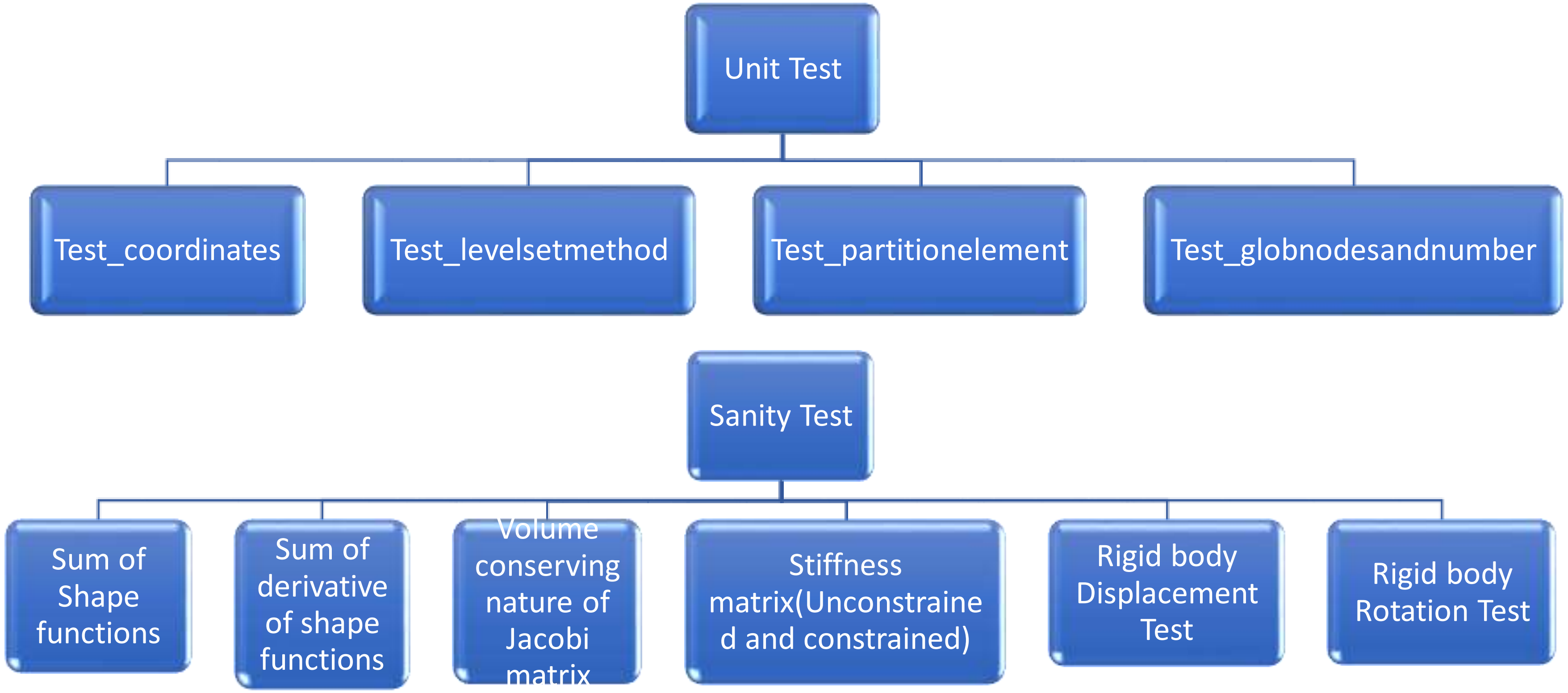


5.Highlights of this project:-

- This project was designed from the ground up, and no working programming code (related to this project) had been viewed or utilized. The project was successfully finished with the assistance of the supervisor's guidance and theories from the book.
- The user can specify the number of discontinuities (max =2, min =1) in this project, which can be a hole, an inclusion, or both.
- As a result, the project provides a user with five provisions (Only one provision can be used at a time). A hole or an inclusion can be distinguished by providing the user with the Young's modulus value.
- The user can apply Plane-stress or Plane-strain condition to solve the problem.
- To recreate the Program as it will appear in commercial software, the user can choose the desired edge to apply Traction force on the plate.
- Similarly, in order to apply Dirichlet Boundary conditions, the user can select the desired edge or corner nodes, making it user-friendly.
- Aside from the task , a provision for applying body forces on the plate has also been provided.

6.Testing of the program:-

→In this project, unit test and sanity test had been done where unit test checks the functions written in the main program and sanity test checks the nature of the numerical model that is implemented in the main program.



6.1 Testing details:-

Unit Test :-

1.Test coordinates

To check the generation of nodal coordinates of an element.

2.Test levelsetmethod:-

To check whether the element is cut by the interface of the discontinuity or not.

3.Test partitionelement:-

To check whether the nodal coordinates of 9 sub-grids have been generated correctly.

4.Test globnodesandnumber:-

To check whether the global nodes numbering for the respective nodal coordinates and for the respective elements have been generated correctly.

Comments:-

All the above unit tests have been successfully passed(Expected result = actual result).

Sanity Test:-

1.Sum of shape functions:-

Sum of shape functions with respect to their Gauss points should be one.

2. Sum of derivative of shape functions:-

Sum of derivative of shape functions with respect to their Gauss points should be zero.

3.Volume conserving nature of Jacobi matrix:-

Jacobi matrix multiplying with the rotation matrix and to check the determinant of Jacobi matrix before and after rotation.

4.Stiffness matrix:-

4.1.Unconstrained rigid body:-

To check the eigen value of the K^{glob}. The number of zero eigen values will be 3.

4.2.Constrained rigid body:-

To check the eigen value of the K^{glob}. The number of zero eigen values will be 0.

5.Rigid body Displacement test:-

To check the translation of the rigid body for the given displacement.

6.Rigid body Rotation test:-

To check the rotation of the rigid body for the any given angle.

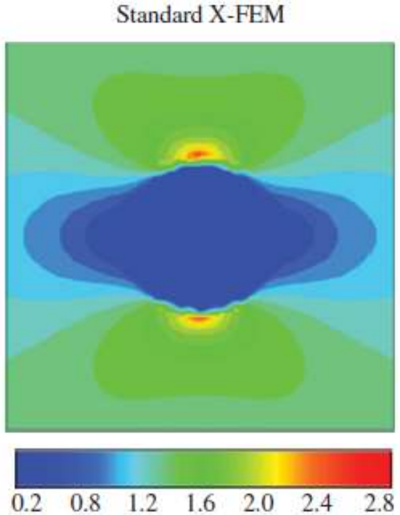
Comments:-

All the above sanity tests have been successfully passed(Expected result = actual result).

7. Details on the tests performed(Validation):-

Expected Output for a plate with the hole (Validation 1):-

Stress contour plot in x-direction (in kg/cm^2)



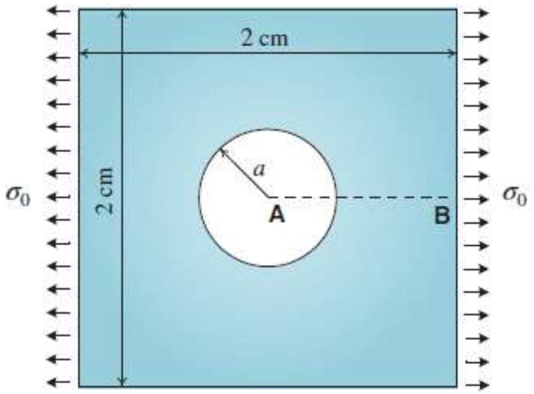
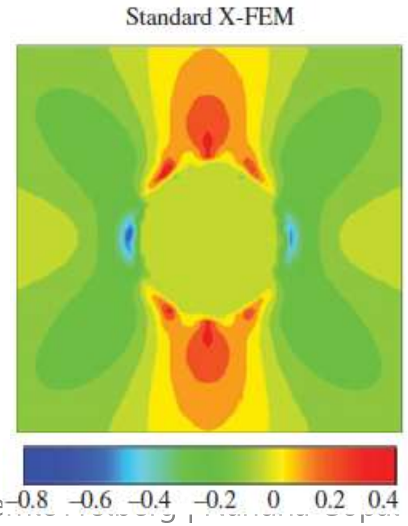


Figure6 : A plate with circular hole at its centre (*Khoei,2014*)

Stress contour plot in y-direction (in kg/cm^2)



- The findings of the displacement contours (in x and y directions) from the written program were compared with the book in validation 1.(Khoei, A. R. (2014). *Extended finite element method: theory and applications*. John Wiley & Sons.)

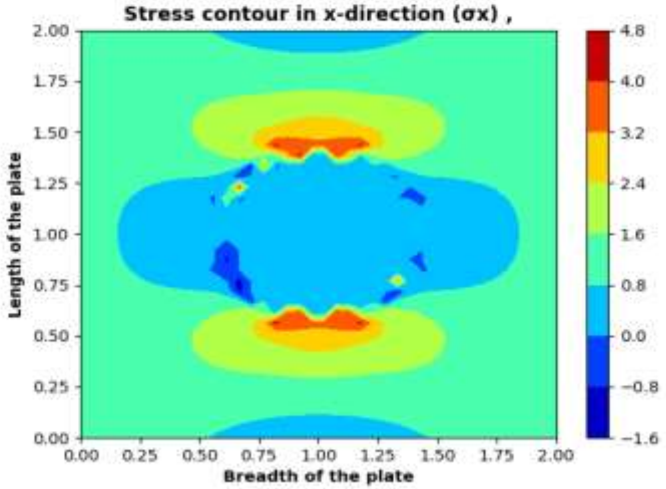
- The images shown in the left are the expected output of the x-directional and y-directional stress contours taken from the mentioned book.

→Inputs given in the book:-

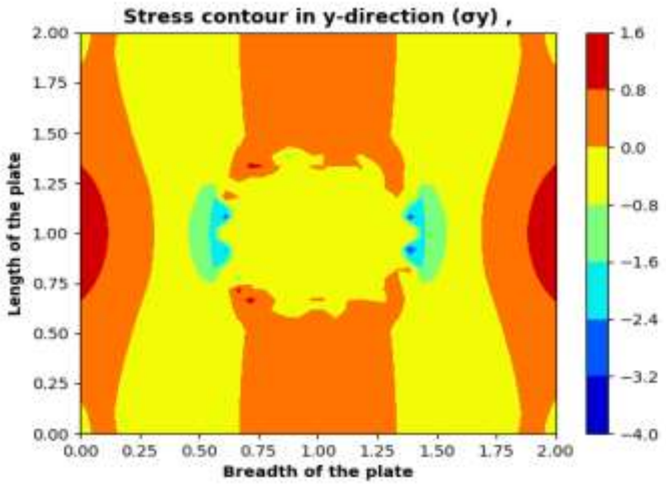
- Square plate of length 2 cm
- Discretization of plate = 30*30 meshes
- E1 = 1*10e5 kg/cm^2 (Young's modulus of the plate)
- E2 = 1*10e2 kg/cm^2 (Young's modulus of the plate)
- Radius of the hole = 0.4 cm at the center of the plate
- Poisson ratio of plate and hole = 0.3
- Plate is subjected to uniaxial Tensile load of 1 kg/cm^2 along x direction.
- Appropriate displacement constraints are only mentioned in the journal article but are not specifically specified or shown where they are added.
- Applying Plane stress or Plane strain conditions to the problem were not mentioned in the book.

Actual Output for a plate with the hole (Validation 1):-

Stress contour plot in x-direction (in kg/cm^2)



Stress contour plot in y-direction (in kg/cm^2)



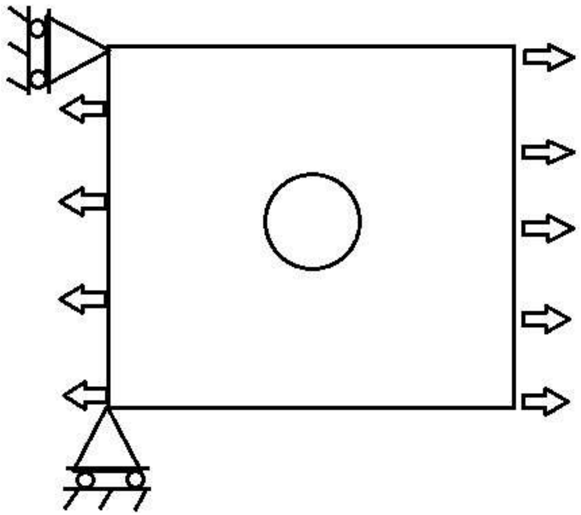


Figure7 : A plate with circular hole at its centre (Validation 1)

- The images/results shown in this slide is taken as a result from the written program **(Programming an XFEM module for investigating the holes and inclusions in a 2D plate).**

- The images shown in the left are the actual output of the x-directional and y-directional stress contours taken from the written program.

Inputs given to the written program:-

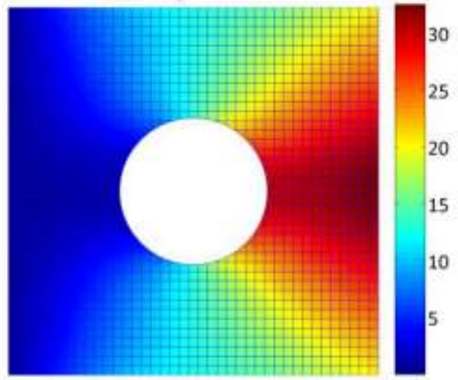
- Square plate of length 2 cm.
- Discretization of plate = 40*40 meshes (1600 elements)
- Poisson ratio of plate = 0.3,Hole = 0.3
- E1 = 1*10e5 kg/cm^2 (Young's modulus of the plate)
- E2 = 1*10e2 kg/cm^2 (Young's modulus of the hole)
- Radius of the hole = 0.4 cm at the center of the plate.
- Plate is subjected to uniaxial Tensile load on x direction = 1 kg/cm^2
- Applied Plane stress condition - (Assumed)
- Applied Dirichlet Boundary conditions on cornernode1 with y-direction fixed and cornernode3 with x-direction fixed. - (Assumed)
- Above 50*50 meshes, it raises singularity error.
- Execution time : 55 sec(approximately).

Possible Errors regarding the accuracy of the results:-

- Improvement needed in the enhanced interpolation of the B-matrix(enhanced).
- Assumed Dirichlet boundary conditions.
- The author has not mentioned about the usage of the partition method for enriched elements.
- Result extraction : Element instead of Node

Expected Output for a plate with the hole (Validation 2):-

Contour plot of the x-direction displacement (in mm)



(a) XFEM

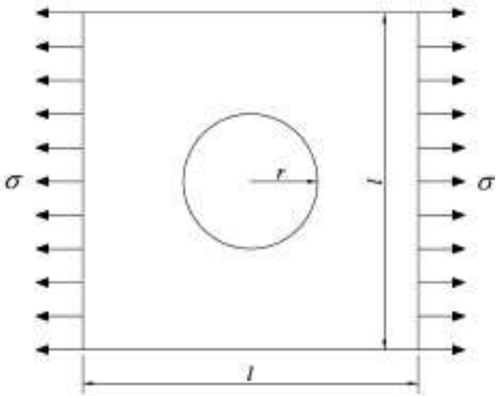
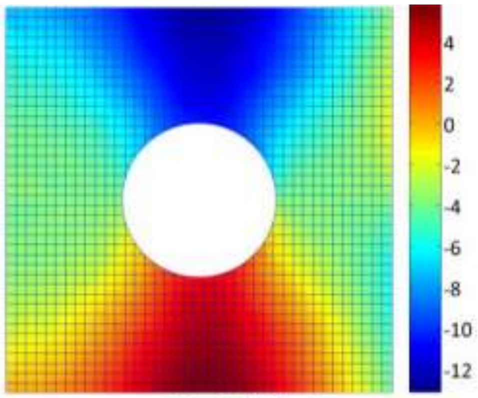


Figure8 : A plate with traction free circular hole at its centre

Contour plot of the y-directional displacement (in mm)



(a) XFEM

- The findings of the displacement contours (in x and y directions) from the written program were compared with the research article in validation 2.(Jiang, S., Du, C., & Gu, C. (2014). An investigation into the effects of voids, inclusions and minor cracks on major crack propagation by using XFEM. *Structural Engineering and Mechanics*, *49*(5), 597-618.).

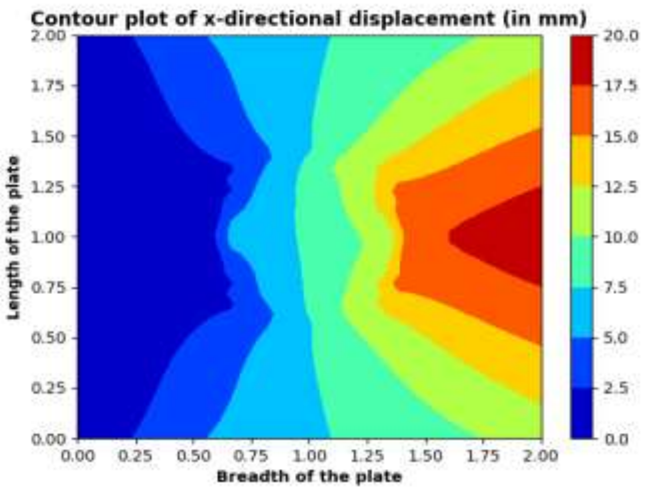
- The images shown in the left are the expected output of the x-directional and y-directional displacement taken from the above research article.

Inputs given in the journal:-

- Square plate of length 2 m.
- Poisson ratio of plate = 0.3, Hole = not mentioned.
- Discretization of plate = 39*39 meshes (1521 elements).
- E1 = 1*10e5 Pa (Young's modulus of the plate).
- E2 = Not mentioned in the paper(Young's modulus of the hole).
- Radius of the hole = 0.4 m at the center of the plate.
- Plate is subjected to uniaxial Tensile load of 1000 Pa.
- Plane strain condition is assumed.
- Appropriate displacement constraints are just mentioned in the journal article but are not specifically specified or shown where they are added.

Actual Output for a plate with the hole (Validation 2):-

Contour plot of the x-direction displacement (in mm)



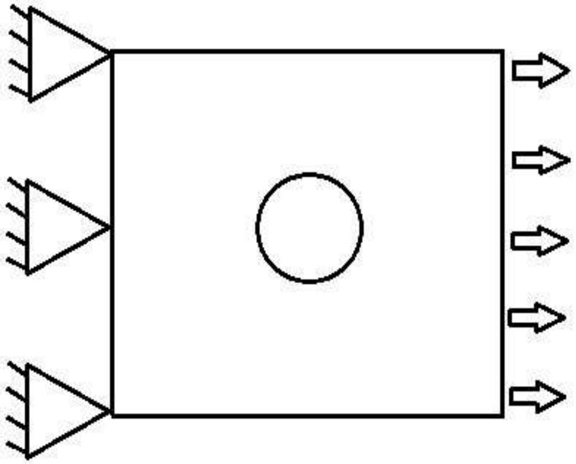
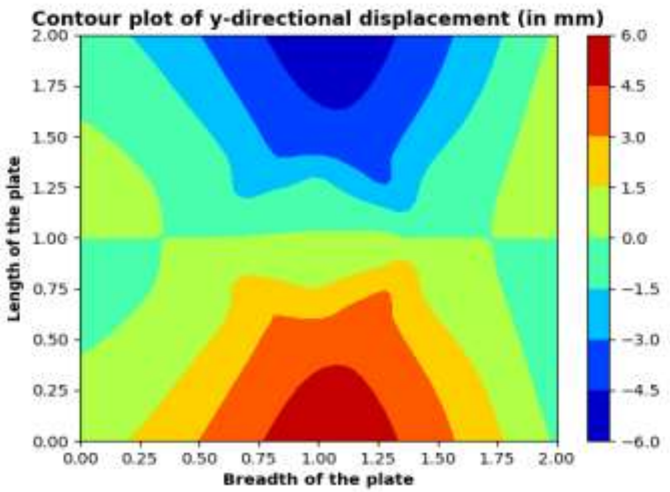


Figure9 : A plate with traction free circular hole at its centre

Contour plot of the y-directional displacement (in mm)



- The images/results shown in this slide is taken as a result from the written program **(Programming an XFEM module for investigating the holes and inclusions in a 2D plate).**

- The images shown in the left are the actual output of the x-directional and y-directional displacement taken from the written program.

Inputs given to the written program:-

- Square plate of length 2 m.
- Discretization of plate = 40*40 meshes (1600 elements).
- Poisson ratio of plate = 0.3,Hole = 0.3 – (Assumed)
- E1 = 1*10e5 Pa (Young's modulus of the plate).
- E2 = 1*10e2 Pa (Young's modulus of the hole). – (Assumed)
- Radius of the hole = 0.4 m at the center of the plate.
- Plate is subjected to uniaxial Tensile load on 'Edge2' = 1000 Pa.
- Plane strain condition is assumed.
- Appropriate displacement constraints have been applied by fixing the 'Edge4' in both x and y directions. – (Assumed)
- Above 50*50 meshes, it raises singularity error.
- Execution time = 42 seconds(approximately)

To improve the accuracy of the results:-

- Improvement needed in the enhanced interpolation of the B-matrix(enhanced).
- Assumed Young's modulus of the hole and Dirichlet boundary conditions.
- Type of partition method : Not a rectangular sub-grid method.
- Result extraction : Element instead of Node

Actual Output for a plate with a hole and an inclusion:-

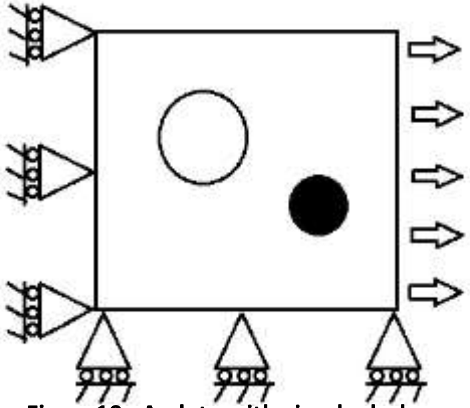
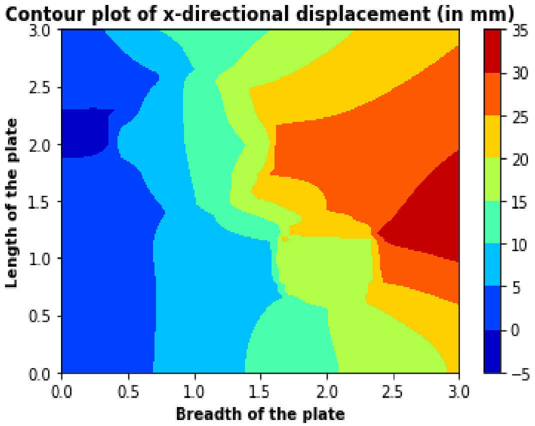
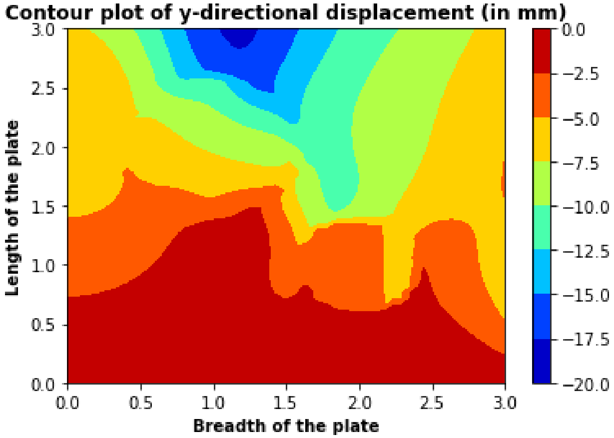
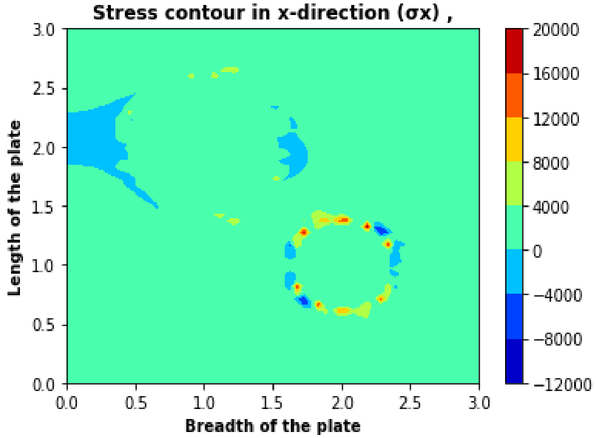


Figure10 : A plate with circular hole and inclusion







Inputs given to the written program:-

- Square plate of length 3 m.
- Discretization of plate = 40*40 meshes (1600 elements).
- Poisson ratio of plate, hole and inclusion = 0.3
- E1 = 1*10e5 Pa (Young's modulus of the plate).
- E2 = 1*10e2 Pa (Young's modulus of the hole).
- E3 = 4.19*10e5 Pa (Young's modulus of the inclusion).
- Radius of the hole = 0.6 m (coordinates x=1,y=2)
- Radius of the inclusion = 0.4 m (coordinates x=2,y=1)
- Plate is subjected to uniaxial Tensile load on x-direction(Edge2) = 1000 Pa
- Plane strain condition is applied.
- Dirichlet Boundary conditions are applied on the Edge 1(constrained in y-direction) and Edge 4 (constrained in y-direction).
- Execution time = 105 seconds(approximately)