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An approach for Coupling FEM & Molecular Dynamics

Satvik Nirwal, Ravi Katukam

[1]IIT KGP,India
[2] Cyient Limited Hyderabad, India

Abstract: The rapidly developing field of nanomechanics is providing new insight in the study of properties of materials by simulating fundamental atomic mechanisms. For broad application of nanomechanics, computational multi-scale methods are necessary to link macroscopic behavior of materials with the underlying atomic processes which are originally responsible for the material behavior.The current work aims to study various multi-scale approaches, with the focus on the linking of Finite Element Method with the Molecular Dynamics Model, developed over time along with their pros and cons and attempts to arrive at the most computationally efficient and effective approach.

This is followed with the identification of the areas of improvement in the selected approach and further continues to model the approach along with the modifications. While achieving the objective, that is the modified approach, the accuracy of the conventional approach may be compromised to some extent but with a good amount of computational space requirement reduction. During the whole process, a detailed study and modeling of conventional Finite Element Method and Molecular Dynamics is also undertaken which are the essential constituent of the Multi-scale model. During Finite Element Analysis, the effect of mesh on the method is also shown and hence, the optimum distribution of elements is obtained from the study.

INTRODUCTION

The introduction of computation in the field of material analysis has reduced significantly the amount of pain, for the engineers, involved in the process. With manual calculations, it would have never been possible to design such complex and large structures, which we sees in everyday life without any feeling of amazement. Such is the power of computation, that it has established itself as a parallel approach to the theoretical studies. It has also proven its effectiveness in both the fields of continuum mechanics and the newly emerging field of nanomechanics.

Nanomechanics is the field where the strength of computation can be observed. It basically deals with the study of interaction of atoms or molecules as one of many other different phenomenon, from where behavior of the material as whole unit originates. Without computational tools, it is impossible to simulate even a very small unit of material. Various methods are used to study nanomechanics using computational science, Molecular Dynamics (MD) is one of these. Although Molecular Dynamics has been able to predict complex physical phenomenon using numerical methods, but it has some limitations in terms of length and time scales.

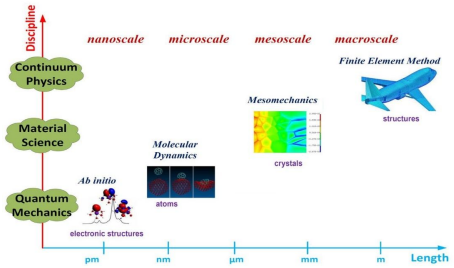
The application of the Finite Element Method (FEM), widely used in the industries and academic research, to a wide and complex range of structures is a reality because of the advent of era of computational technology. It has made the work of engineers a lot easier. But the accuracy of the method, while dealing with certain specific kind of problems, cannot be trusted completely. This gives indication that something is not right with the way, the problem is being dealt with.

Different Scales of Analysis

It can be observed that computational techniques are essential component of both microscopic and macroscopic analysis of materials now-a-days. Depending on the objective of the analysis, we apply different scale approach, for example, to study stress distribution in large aircraft components, we cannot afford to go for analysis using microscopic approach as it neither desirable nor affordable for the commercial industry, while to study crack propagation in a very small region, it is advised to go for microscopic analysis of the region rather than using macroscopic methods like FEM which does not have required level of accuracy.

The above discussion highlights the importance of proper scale of analysis to achieve required accuracy and efficiency. Wrong choice of scale during the material analysis can lead to confusing and misguiding results. We can broadly classify different scales involved in the material study as-

i. Nano-scale
ii. Micro-scale
iii. Macro-scale



At different scales, the nature of basic laws of physics responsible for the material behavior also changes (continuum for macroscopic while discrete atomic physics for atomic scale) and hence different methods are used for the analysis, as shown in the above figure. A brief description of the various methods is given below:

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a) **Finite Element Method:** This method is generally used in analysis of macroscopic structures. It is based on principles of continuum mechanics which at macroscopic scale usually yields results of sufficient accuracy. Most of the industries prefer this method as it is computationally efficient, inexpensive as compared to others and effective enough for the industrial requirements. The accuracy deficiency can be dealt by introducing factor of safety in the analysis.

But this has also got certain limitations. Since the mechanics involved is continuum in nature, it cannot model the phenomenon which involves effects of defects in lattice, cracks or some other atomic scale factors (discrete nature of material atoms has to be considered).

b) Molecular Dynamics: This method is used for analysis at micro or nano-scale. It is based on the fact that material behavior originates from the molecular or atomic behavior in solids (neglecting intra-molecular degree of freedom). This approach predicts the trajectories of molecules or atoms by using simple Newton's second law of motion. In the process, for calculation of inter-atomic force distribution interatomic potential is utilized. Some of the commonly used interatomic potentials are Lennard Jones 6-12 potential, Morse potential and Embedded Atom Model (EAM) potential. It makes this approach a suitable candidate for application in areas like study of composite behavior, crack propagation etc. There is no doubt that this method provides extra accuracy over FEM.

Molecular Dynamics approach is expensive as it requires a lot of computational resources. With the present set of resources, it can be performed only over a very small domain. This sets a check on this approach and it is the basic reason why industries do not usually prefer it for general analysis, unless required specifically. Also it faces some difficulties in distribution of external load over the whole domain.

c) Tight Binding Method: This is one of the finest method in terms of resolution. It is based on the principles of quantum mechanics which is very interesting field in itself. This method calculates the electronic structure by assuming wave functions. The results obtained from this method are very accurate but the computation process is quite intense which makes this method very expensive.

Analysis at that scale is not required for industrial purposes. This restricts the usage of this method for research studies only. The above discussion shows that for different scale of analysis different methods are used which follows different principles. Various methods specified above have certain limitations as briefly described and hence cannot be applied in all the circumstances. This poses a problem if a reasonably large structure with certain defects, which can be modelled properly in macroscopic methods, is to be analyzed. Here, 'multi-scale approach' comes to our rescue.

Multi-scale Approach

In multi-scale approach, different sections or domains of the same structures are analyzed on different scales as per requirement. This leads to effective and efficient analysis of the structure as compared to any particular method. The results thus obtained are better qualitatively and the process is less expensive compared to any method available.

This solves our problem to some extent, but the accurate and smooth transfer of information between different scales is very difficult to achieve. It requires a mechanism which can do this without being computationally inefficient. This phenomenon of transferring the information between different scales using a proper technique is popularly known as *'Multi-Scale Modeling'*. The present work attempts to study various multi-scale modelling techniques and select better technique for the coupling of Finite Element Method (FEM) with the Molecular Dynamics (MD) model.

FEM is widely used in the industry but it has got certain limitations and cannot be applied everywhere, for example crack propagation, lattice defects etc. Similarly MD model can be used for the above stated cases but it requires large amount of computational resources. This makes the application of MD over whole structure infeasible. Thus using multi-scale modeling, only critical part is analyzed using MD while the entire remaining structure is studied using FEM which makes the analysis more qualitative and less expensive as compared to individual approaches.

Thus, multi-scale modelling can save a lot of time and resources for complicated and more accurate material analysis. As in our case, if FEM and MD approaches are effectively combined, they could help solving some of the current problems in Aerospace and Material science like behavior of composites and polymers, crack propagation and its effect on the structure etc. This can greatly improve the quality of the material analysis performed in the industry.

Outline of the work

Firstly a brief study over various available multi-scale modeling techniques is undertaken. In the study the basics of the approaches and their limitations are presented. This is followed by the selection of a particular technique for the coupling of FEM and MD. The detailed description of the selected multi-scale model (ESCM) is presented. Some improvements are also suggested in the conventional model. Results obtained by modifying the model with the suggested improvements are also shown for the case of a simple 2D plate.

During this process, FEM and MD tools are developed to obtain the results from the multi-scale model. The verification of the developed model is done by using software like Nastran-Patran. A brief study about the effects of mesh on the results of FEM is also undertaken as a matter of interest.

At last, factors affecting the obtained results from the modified form of the conventional model are stated in order to account for the discrepancy in the results obtained.

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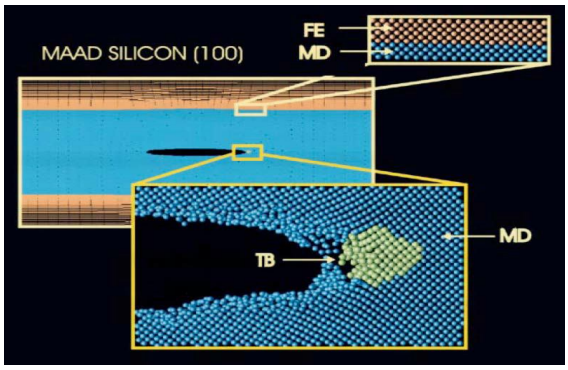
MULTI-SCALE MODELING:

A brief discussion about the Multi-Scale modeling approach is already presented. In the present work the focus is on selecting a suitable model for coupling of FEM with MD. MD and FE methods are well suited to a particular level of accuracy on atomistic and continuum simulations, respectively. In general, MD cannot be used for macro-scale problems due to the restrictions on the number of atoms that can be simulated simultaneously, along with the timescale limit. On the other hand, usage of FE method for atomic scale problems is not accurate for many reasons mainly because continuum mechanics assumes that the substance of body is distributed continuously throughout the space of body and lacks atomic degrees of freedom. These inherent limitations make connecting these two methods essential but also



challenging. It must be pointed out that MD does not have any electronic degrees of freedom.

Challenges in Coupling of FEM and MD

The basic difference lies in the nature of physical laws followed in both methods. FEM is entirely based on continuum mechanics while MD derives its nature from observation of molecular behaviour. These differences leads to many problems in communication of information between these methods during the Multi-scale simulation. Some of the major challenges are listed below:

- The very nature of displacements is different in both cases. In FEM, the displacement is averaged (continuous) while in MD the displacement is discrete and can take any value without continuity.
- The nature of oscillation is also different. The oscillation are slow and swift in FEM while they are fast in MD model. This leads to difference in the order of velocities involved in both methods.
- Also the nature of forces is different. Forces are continuous and distributed at the continuum level (FEM) while they are discrete at atomistic scale. Thus the force has to be evaluated for each molecule or atom in MD while they can be easily predicted in FEM.
- Another major and most important difference is that of the time scale involved. In FEM, it is of order of microsecond or millisecond while it is of the order of femtosecond in case of MD. Thus MD system can be simulated at maximum for few microseconds which make it not useful for real life simulations.

Different Multi-Scale Methods

A literature survey has been done on the various Multi-Scale models developed till now. A brief summary of each of those models is presented here.

a) Macroscopic Atomistic Ab-initio Dynamics (MAAD): This method is one of the earliest successful methods developed for Multi-scale modeling and received a lot of attention. It was developed by Abraham and his colleagues in around 1999. The fundamental idea is to make concurrent links between tight-binding (TB) method, molecular dynamics (MD), and finite element method (FEM). In this method, tight binding method is used for quantum mechanics level degrees of freedom. Molecular dynamics is used for the representation of atomistic degrees of freedom. Finite element method is used for the deformation of continuum mechanics. Here, all three simulations run at the same time, and dynamically communicate required information between the simulations. The interactions among three analyses are taken into account by the total Hamiltonian of the system.

In this model, 'handshake' region was adopted to couple regions with each other in *FE/MD*. A very thin hand shake region is used. FE mesh is graded down to the atomic size for the reduction of wave reflection between MD and FE. However, when connecting molecular dynamics and continuum mechanics by using MD simulation and FE method respectively, this technique uses the atomic scale mesh size for FE.

Limitation

Simulation time of FE slows down to picosecond to match the MD time step when the mesh is graded down to atomic level. The other issue is that atomic scale FE simulation is physically unreasonable because the constitutive equation of FE is based on continuum mechanics. Since, time step in FE region depends on the element size, the atomic sized mesh makes the time step too short for realistic engineering problems.

Also there is reflection of short wavelength at the FE/MD interface as atoms on FE side are stationary while that on MD side are constantly vibrating.

b) Quasi Continuum (QC) Method: Another pioneering approach for multi-scale methods is the quasi-continuum (QC) method by Tadmor (1996). The QC method is an approach coupling continuum mechanics with atomistic simulation for the mechanical response of poly-crystalline materials at zero temperature. This is one of most popular method in multi-scale modeling.

The QC method is based on an entirely atomistic description of the material domain. To reduce the computational cost, two assumptions are adapted: one is the reduction of degrees of freedom, and another is the Cauchy–Born rule: in a crystalline solid subject to a small strain, the positions of the atoms within the crystal lattice follow the overall strain of the mediums. The Cauchy–Born rule assumes that the continuum energy density W can be obtained by using an atomistic potential, with the link to the continuum being the deformation gradient F given by:

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$F = 1 + (du/dX)$ ……(1)

Where u is the displacement, dX is an undeformed line segment.

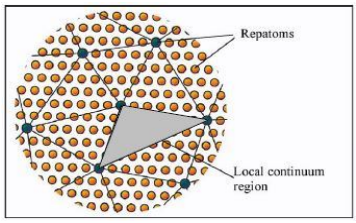
By using the Cauchy–Born rule, a continuum stress tensor and tangent stiffness can be acquired from the interatomic potential W, which allows the usage of nonlinear FE techniques. The continuum stress tensor and tangent stiffness are given by:

$P = \partial W / \partial F$ ……(2)

$C = \partial^2 W / (\partial F^T \partial F^T)$ …..(3)

Where P is the first Piola–Kirchoff stress tensor and C is the Lagrangian tangent stiffness.

The particular representation is determined by the local deformation gradient and dictates a small fraction of the atoms (called representative atoms or "repatoms"). In this approach, the non-local repatoms are used to represent the atomistic behaviors, and the local repatoms are used to simulate the continuum domain by using the Cauchy–Born rule in the FE method as shown in the figure.



Limitations

Although QC method suggested a new approach for multi-scale modeling, this method suffers from the same issues as MAAD that are the wave reflection and the total simulation time limit.

In this method, even though Cauchy–Born rule connects atoms in MD region with repatoms in FE, in which the mesh size of FE gradually increases from MD region, the wave reflection still exists in MD region. The result leads to spurious energy accumulation in MD region, non-physical heating of the crystal in the MD region, and as a result the solution in MD region becomes unreliable. Moreover, since this method is implemented in MD and FE regions simultaneously, the time step of MD dominates the total simulation time, which is very short for any practical engineering problem.

c) Bridging Domain Method: Xiao and Belytschko (2004) have developed this method for coupling of molecular dynamics and continuum mechanics. In this approach, the system consists of three domains: Ω_{MD} (molecular dynamics), Ω_{CM} (continuum mechanics), and Ω_{HS} (hand shake region) which can be seen in the figure. The main idea of the model is using a linear combination of Hamiltonian of MD and FE region in the hand shake region, Ω_{HS}. Hamiltonian is defined by:

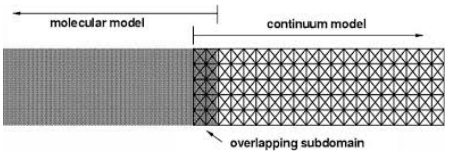
$H = (1-\alpha)HMD + \alpha HCM$ ……(4)

Where the parameter $\alpha = 0$ in Ω_{MD}–Ω_{HS} region, and $\alpha = 1$ in Ω_{CM}–Ω_{HS} region while $\alpha = [0,1]$ (linear) in Ω_{HS}.

The energy within the hand shake region goes from entirely atomistic at MD boundary to entirely continuum at FE boundary. The effect of this energy transition is that short wavelength atomic scale energy is filtered but results have shown that a minimum hand shake distance is required for the method to eliminate wave reflection effectively.

Limitation

The minimum hand shake distance in this method is relatively long, as a result increasing the computational cost and decreasing the size of MD zone.



d) Bridging Scale Method: This method was developed by Wagner and Liu (2003), and Park and Liu (2004). The basic idea is to resolve the total displacement $u(x)$ in terms of course scale $\bar{u}(x)$ and fine scale $u'(x)$ at the position x. The coarse scale is governed by the continuum mechanics and simulates the entire field, while the fine scale is used to simulate the region of high interest is governed by molecular dynamics.

Bridging scale method starts from an entire molecular system. For better efficiency, the system area of MD is reduced from the entire region to a small area of interest. An entire molecular system can be changed into the reduced MD system along with external forces that act on the boundaries of the reduced lattice. The latter represents the combined effects of all the atomistic degrees of freedom accounted for by using the generalized Langevin equation (GLE). Effect of using GLE with FE mesh is the dissipation of small wavelength which FE cannot capture due to its mesh size.

This approach does not scale down the mesh of FE to atomic size and thus provide different simulation time scales for both FE and MD. Thus the coarse scale variables can evolve on different time scale than the fine scale variables. The wave reflection results are also good with this method.

Limitations

This method does not have the problem of wave reflection and time scale dependency. But the computations involve are complex in multiple dimensions and hence, brings additional computational cost in MD simulation.

Embedded Statistical Coupling Model (ESCM)

This is rather a new approach to MD-FEM coupling, developed by E. Saether (2009), which is based on a restatement of the standard boundary value problem used to define a coupled domain. The method replaces a direct linkage of individual MD atoms and finite element (FE) nodes with a statistical averaging of atomistic displacements in local atomic volumes associated with each FE node in an interface region. The FEM and MD computational systems are effectively independent and communicate only through an iterative update of their boundary conditions.

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With the use of statistical averages of the atomistic quantities to couple the two computational schemes, the developed approach is referred to as an embedded statistical coupling method (ESCM). ESCM provides an enhanced coupling methodology that is inherently applicable to three-dimensional domains, avoids discretization of the continuum model to atomic scale resolution, and permits finite temperature states to be applied.
This is the model which is being followed during this work. The detailed description and areas of improvement are discussed here.

Why ESCM?
The ESCM model has got many advantages over the other multi-scale models some of which are listed below-

- While most of the methods are based on one to one relation between FE nodes and atoms (Direct coupling) which makes resolution of FE mesh to atomic level necessary, it can be avoided in ESCM.
- The time scale of FE domain and the MD region are different and hence, the variables of both domain can evolve on their own time steps.
- It involves an iterative procedure at the interface between MD displacement and the FE reaction forces which ensures continuity at the interface.
- It can be used for 3D structures and for any temperature while some of the methods require the analysis to be performed at 0 K.
- Less computational space is required as compared to other methods for the same structure as simple statistical averaging is involved.

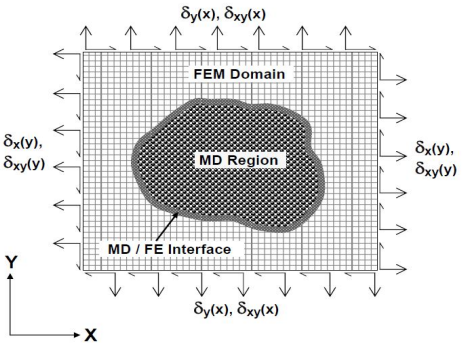
ESCM Model and Improvements

ESCM approach is focused on coupling of MD-FEM system. The approach is based on solving a coupled boundary value problem (BVP) at the MD/FE interface for MD region embedded within a FEM region. Since, this method uses statistical averaging over both time and volume in atomistic sub domains at the MD/FE interface to determine nodal displacement boundary conditions for the continuum FE model, it is efficient computationally as compared to other methods. These enforced displacements, when applied to FE analysis, generate interface reaction forces that are again applied as constant traction boundary conditions between updates of the FEM solution to the atoms within the localized MD sub domains. Thus, the present approach relates *local* continuum nodal quantities with *nonlocal* statistical averages of atomistic quantities over selected atomic sub domains.

An iterative procedure between the MD statistical displacements and the FEM reaction forces ensures continuity at the interface. In this way, the problem of redefining continuum variables at the atomic scale is avoided, and also the time and length scales between the MD region and FEM domain are independent.

With the emphasis of using statistical averages to couple the two computational schemes, the developed approach is identified as a *statistical* coupling (SC) approach. Based on the SC approach, the developed MD-FEM coupling method is referred to as the embedded statistical Coupling Method (ESCM).

ESCM Model
The ESCM approach is developed to reduce computational costs incurred while simulating “large” volumes of material by embedding an inner atomistic MD system within a surrounding continuum FEM domain. In principal, the shape of the atomistic region may be arbitrary as shown in figure. However, for simplicity, the special case of a circular region is utilized in the present work. Similarly, although any constitutive behavior may be assumed for the FEM domain, the present study considers a linear elastic continuum.



This model can really be helpful while studying the processes like void nucleation and crack growth in a structure, impact of crack on material strength, behavior of composite materials, effect of lattice defects on the entire material properties etc.

The structure of the ESCM model consists of four regions:

1) Inner MD Region
2) MD/FE Interface region
3) Surface MD region
4) FEM domain

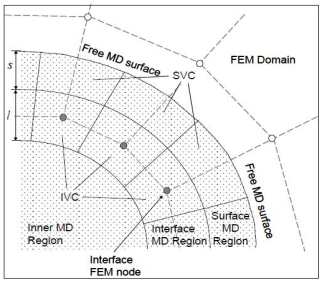


Figure 2. Structure of the MD/FE Interface in the ESCM approach.

These four regions are depicted in figure shown here. Interface region is the region where MD and FE domains are superimposed. Surface region does not interact with FE domain but it compensate for the atomic free surface effects.

The individual regions will be discussed in details in next few sections.

1. Inner MD and the FEM domain:
The Inner MD Region is used to model material phenomena at the atomistic level. This is basically the region of high interest in the simulation and most of the computational space is utilized in this region. It should be large enough to ensure a statistically smooth transition from a continuum to an atomistic representation while modeling any of the types of processes (e.g., dislocation formation, void nucleation, or crack propagation) that are required by the simulation.

The Inner, Interface, and Surface MD regions together constitute the complete MD system. Here it is important to emphasize that the partitioning of the MD system into different regions is not a physical separation of the system.

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An atom assigned to a particular location freely interacts with atoms in its interaction neighborhood that may reside in a

different region. Thus, the overall simulation is performed using any conventional MD technique without any imposition of direct kinematic constraints. The only difference between the three MD regions is that, while the atoms in the Inner MD Region are subject only to their interatomic forces, the Interface and Surface MD Regions serve the added purpose of facilitating the application of external forces involved in the ESCM procedure.

Here, the addition of a FEM domain permits a large reduction in the computational cost of simulations by replacing the atomistic representation with a continuum model in those parts of the system where the deformation gradients are small and atomic-level resolution is not necessary.

The current application uses the FEM domain to simulate an extended material model such that the elastic deformation and load transfer due to applied far-field boundary conditions are accurately transferred to the Inner MD Region. The continuum field is currently assumed to be static with linear elastic material properties but other applications of ESCM might require the incorporation of nonlinear material behavior, such as plasticity or general dynamic response, where nonlinear processes generated in the Inner MD Region can be propagated into the continuum.

2. MD/FE Interface Region:

The main role of the MD/FE Interface is to provide a computational linkage between the MD region and FEM domain. The atoms that surround a given FE node at the interface are partitioned to form a cell in the Interface MD Region, called an interface volume cell (IVC) as shown in the figure representing the ESCM model. The IVCs compute averaged MD displacements at their mass center that are then prescribed as displacement boundary conditions to the associated interface finite element nodes. The IVCs need not coincide in size or shape with the finite element to which the FE node belongs.

In the model, IVCs are formed through a Voronoi-type construction by selecting those atoms with a common closest finite element node. Typically, one finite element at the interface encompasses a region of several hundred to several thousand atoms. A lower bound for the number of atoms associated with each finite element node is determined by the requirement of obtaining a minimally fluctuating average of atomic displacements and minimizing the magnitude of generated gradients in the MD region bordering the FEM domain. With an effective average at this scale, the discreteness of the atomic structure is homogenized enough so that the FEM domain responds to the atomistic region as an extension of the continuum.

During the coupled MD-FEM simulation, a spatial average within each k^{th} IVC is performed to yield the center of mass displacement, $\vec{\delta}^{MD}_{CM,k}$, which is further averaged over a certain period of M MD time steps to yield the statistical displacement vector, $\vec{\delta}^{MD}_{I,k}$

$$\vec{\delta}_{I,k} = \langle \vec{\delta}_{CM,k} \rangle_t = \frac{1}{M} \sum_{j=1}^{M} (\vec{r}_{CM,k}(t_j) - \vec{r}_{CM,k}(0)) \quad \text{.....(5)}$$

Here, $\vec{r}_{CM}(t_j) = \frac{1}{N_k} \sum_{i=1}^{N_k} \vec{r}_i(t_j)$ is the center of mass of the k^{th} IVC containing N_k atoms at positions $\vec{r}_i$ at time t_j of the j^{th} MD step. The mass center displacement, $\vec{\delta}_{CM,k}$, in Equation (5.1) is calculated relative to the initial zero-displacement position of the k^{th} IVC, $\vec{r}_{CM,k}(0)$.

In turn, the IVCs distribute reaction forces from the interface finite element nodes as external forces applied to the corresponding atoms within the IVC.

3. Surface MD Region:

As discussed above, reaction forces are obtained from FE analysis which are applied on the MD model. In order for the MD domain to deform freely in response to these applied reaction forces, it is modeled using free surface boundary conditions.

However, the existence of a free surface introduces several undesirable effects in the MD system. First, it creates surface tension forces that must be removed to avoid distorting the MD response. Second, because atoms at or near the free surface do not have a complete set of interacting neighbouring atoms, the coordination number of the surface atoms is reduced so they are less strongly bonded to the surrounding atomic field than those within the interior. Under sufficiently large reaction forces, these atoms may be separated from the surface layer causing a surface degradation within the MD domain.

To mitigate these free surface effects and to stabilize the atoms in the Interface MD Region, an additional volume of outlying atoms constituting a Surface MD Region is introduced as shown in Figure representing the ESCM model. While the Surface MD Region eliminates the free surface effects within the Inner MD region, it also introduces an undesirable fictitious stiffness that elastically constrains the deformation of the Inner MD Region. The separate effects of surface tension and the fictitious stiffness cannot be computed independently. However, their combined effect may be defined as a resultant force, $\vec{F}_s$, which acts at the boundary between the Surface MD Region and the Interface MD Region, and is given by the sum of two components expressed as

$$\vec{F}_s = \vec{\xi} + \vec{\tau} \quad \text{....(6)}$$

Where $\vec{\xi}$ - Elastic reaction of surface region under deformation

$\vec{\tau}$ - Force from the surface tension

To mitigate both the surface tension and the elastic response of the Surface MD region $\vec{F}_s$ needs to be compensated. In the ideal case, when $\vec{F}_s$ is fully compensated, the Surface MD region acts as if it possesses zero stiffness and experiences no

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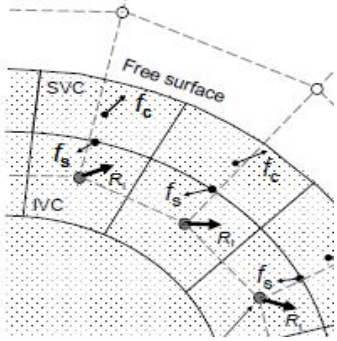
surface tension, thereby mitigating spurious influences on the Inner MD Region.



For the purpose, Surface MD Region is subdivided into a number of SVCs. It helps to follow the variations of $\vec{f}_s$ along the perimeter of the Interface MD region. For convenience, the partitioning of SVCs can be made to follow the IVC partitioning of the Interface MD Region. The resultant force is then calculated individually for each SVC. To compensate, $\vec{f}_s$, a counterforce, $\vec{f}_c$, is computed along the IVC/SVC interface and then distributed over the atoms of each SVC in a similar manner as the nodal reaction forces are applied to the IVCs of the Interface MD Region as shown in the figure.

MD-FEM Coupling Algorithm

The MD-FEM coupling in ESCM is achieved through an iterative equilibration scheme between the MD region and the FEM domain. In this scheme, iterations begin with displacements at the MD/FE Interface that are calculated as statistical averages over the atomic positions within each IVC and averaged over the time of the MD analysis. These average displacements are then imposed as displacement boundary conditions on the FEM domain. The resulting FEM BVP is then solved to recover new interface reaction forces resulting from the applied interface displacements and any imposed far-field loading.

The new interface reaction forces are then distributed to the atoms in the IVCs, thus defining new constant traction boundary conditions on the MD system. Between the FEM solution updates, the traction boundary conditions are constant and applied to the MD region to ensure that the elastic field from the FEM domain is correctly duplicated in the atomistic region. The MD-FEM iteration cycle repeats until a stable equilibrium of both displacements and forces between the atomistic and continuum material fields is established at the interface. The whole algorithm is shown above in the form of flowchart.

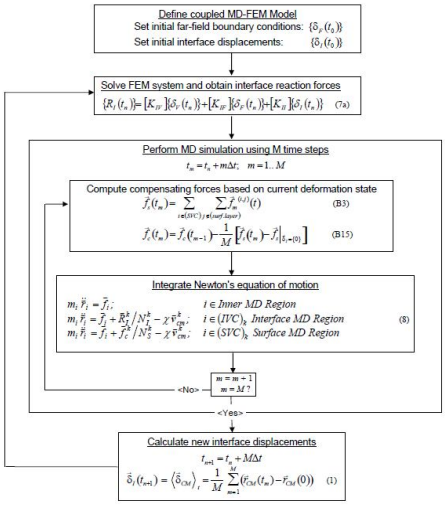


Figure 4. Flowchart summarizing the coupled analysis procedure.

Improvements in the ESCM Model

ESCM model has proven itself to be an efficient and effective model by overcoming limitations of other methods and utilizing less computational space, as compared to other methods, at the same time. But the method still requires a lot of computational resources to be applicable for large scale industrial purposes.

Although the method is optimized for its objective but still it has got some areas where improvements can be made. One such area is the calculations involved in surface forces compensation. An extra layer of atoms has to be added in the MD domain of conventional ESCM model, to counter the surface forces involved, while simulating the MD domain. This induces an extra pressure on the computational resources as force matrix has to be generated for these extra atoms.

This can be avoided if some mechanism other than introducing extra atoms is used. On a primitive thought, the periodic boundary conditions (PBC) may be used as the mechanism to avoid surface forces at the first hand. This can greatly reduce the large computations involved in the surface MD region of conventional ESCM model. Although the accuracy of the model may suffer in introducing the PBC, but the reduction in computation time may play an effective role.

In the present work, it will be tried to study a multi-scale model of a simple 2D plate using the modified approach. Then the reduction in accuracy along with the reduction in the computational space and time, can be observed for that case. If the results are sufficiently accurate, then different models can be used to check the viability of the proposed modification. If confirmed this play a key role in the efficient multi-scale modeling.

Results and Conclusion

In this section, a simple 2D plate of Aluminium is analyzed using the ESCM model with the modifications proposed in the previous chapter. The model has an embedded circular MD region at the center of the plate while the rest of the region is analyzed using FEM (FEM domain). Thus the net FEM domain looks like a plate with a hole kind of situation and the MD domain is a circle of a particular radius.

First the meshing for the FEM part is done after fixing the dimensions of the 2D plate. Special focus has been given on the mesh quality perspective as it is very important. Since, FEM tool and MD tool are already developed, as discussed in the previous chapters, Multi-scale analysis can be performed directly after the meshing is done. Here, it must be emphasized that the parameters in MD model are very near to that of Aluminium parameters but not that much accurate.

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The focus of the analysis is to reach to an equilibrium state and compare the stress pattern thus obtained with that obtained from simple FEM analysis.

In the following sections, first dimensions of the coupling model (2D plate in this case) are presented. Then FEM analysis of 2D plate with a hole at the center is presented along with a brief discussion about the mesh quality. This is followed by the results obtained from the Multi-scale analysis of the plate and the critical analysis of the results.

Coupling Model

The structure on which the coupling is done in the present work is a simple 2D Aluminium plate. The dimension and other required parameters for the MD and FEM analysis are

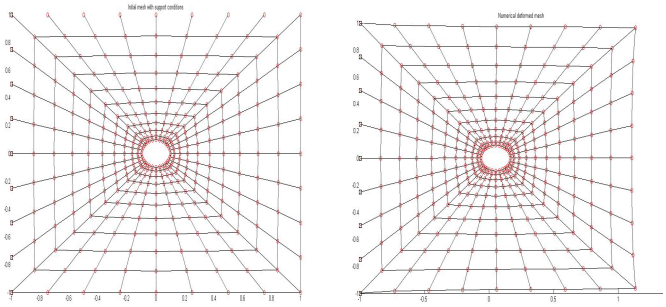
Parameter	Value
Length of plate	4000 A^o
Breadth of plate	4000 A^o
Lattice parameter	4 A^o
Radius of MD Domain	40 A^o
Number of atoms	960
Young's Modulus	70 GPa
Poisson's Ratio	0.33
Material of Plate	Aluminium
Force on Right (Nodal force)	0.01 wton

The FEM domain in the coupling model selected look like a 2D Aluminium plate with a hole. Thus first FEM analysis of 2D plate with a hole at center is done and the results are compared with the one obtained from Nastran-Patran to make sure the quality of FEM tool in the case. This is followed by a discussion on the mesh quality. The dimension of the plate are given below:

Dimension of the plate (square)	2 m	Young's Modulus	70 GPa
Radius of the hole	0.1 m	Poisson's Ratio	0.33

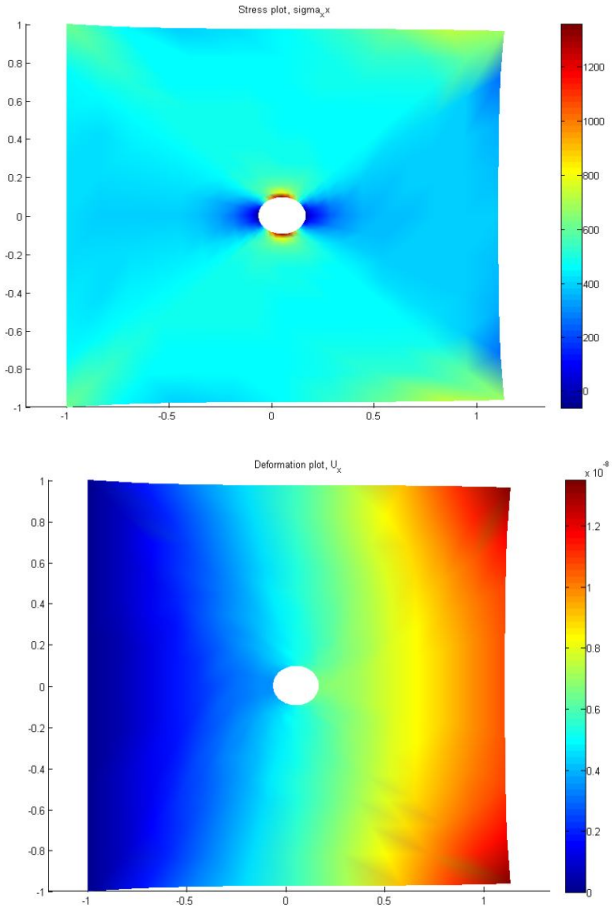
FEM Analysis of 2D Plate with hole

During the FEM analysis of 2D Aluminium plate with a hole at center, of the dimensions discussed above, first step is to perform the meshing of the structure. The mesh used here has 10 elements in radial direction while 8 elements along each edge. Thus the total number of elements in the mesh are320. For better view, the meshing of the plate before and after the deformation respectively are shown below:



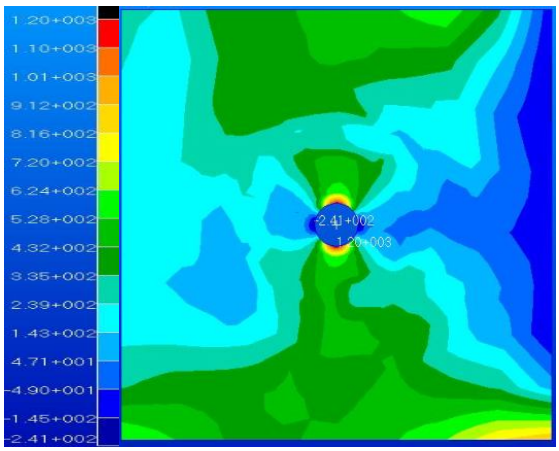
Stress and Displacement distribution

The stress and displacement distribution obtained for the above case using the FEM tool developed is shown here. The results are then compared with the one obtained from the Nastran-Patran tool to check the applicability of FEM tool for use in multi-scale modeling.



Stress and Displacement pattern respectively (from FEM tool) are given below:

Stress and Displacement pattern respectively (from Nastran-Patran) is shown below:



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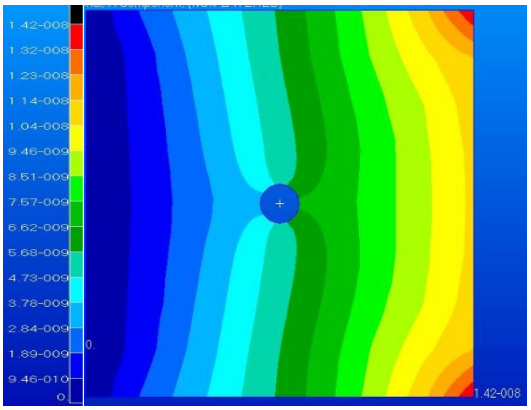


The above results shows a bit difference in color pattern which is mainly due to difference in meshing of the Nastran-Patran and the FEM tool model. But order of magnitude and stress concentration regions are in agreement. Thus the FEM tool can be used in the Multi-scale model with sufficient accuracy. The variation in maximum stress and displacement is shown for the comparison-

From the stress plot,
Maximum stress = 1200 N/m^2 (From the Nastran analysis)
Maximum stress = 1360 N/m^2 (From the matlab code)
Error = 13.3 %

From the displacement plot,
Maximum displacement =1.42e-8 m (From the Nastran)
Maximum displacement = 1.35e-8 m (From the matlab code)
Error = 4.8%

Mesh Quality

The mesh quality depends on the number of elements, distortion factor and aspect ratio (ideally it should be ~1). Out of these distortion factor can be ignored as the order of deformation is very small. For the case of plate with hole, the factors affecting the mesh quality are: number of elements along radial direction, number of elements along circumference and gradient of element length along radial direction.

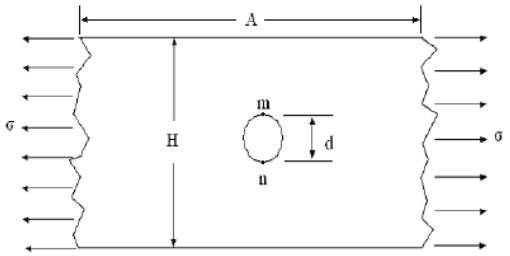
To properly observe the quality of mesh, stress concentration factor has an important role to play. Stress concentration factor, K_{tg}, is defined as the ratio of maximum stress to the reference stress (average stress along the entire cross section).

$K_{tg}=\sigma_{max}/\sigma$ ……(7)
Where, σ_{max} = maximum stress
σ = gross stress along the cross section of the plate

According to Pilkey and Pilkey, for 2D plate with a hole under biaxial loading as shown in the figure, the theoretical value of stress concentration can be formulated as

$$K_{tg} = 0.284 + \frac{\frac{d}{H}}{1-\frac{d}{H}} - 0.600\left(1-\frac{d}{H}\right) + 1.32\left(1-\frac{d}{H}\right)^2$$

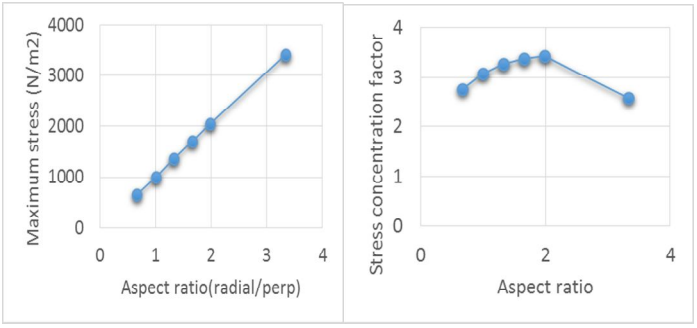
…… (8)



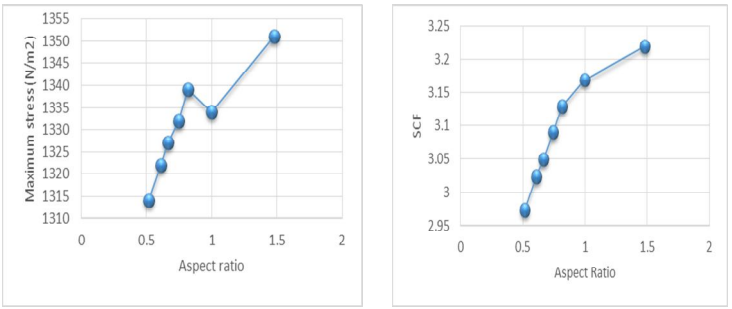
For the present case, H = 2 m, d = 0.2 m
Hence, theoretical value of, K_{tg} = 3.035

Thus the aim of the study is to make the aspect ratio to be around unity, stress concentration factor to be around the above specified theoretical value.

Changing the number of element along circumference
The number of elements along the circumference are changed while the element along the radial direction are same as above (=10). This change leads to change in aspect ratio as well as number of elements in the mesh. The observed pattern is shown here –



Changing the number of elements along radial direction
Now the number of elements along circumference are kept



constant while the number of elements along radial direction are changed. This lead to change in aspect ratio which is plotted below. It is to be noted here that the number of elements are nearly the same.

- For number of elements (on a particular edge) along the perpendicular direction = 8

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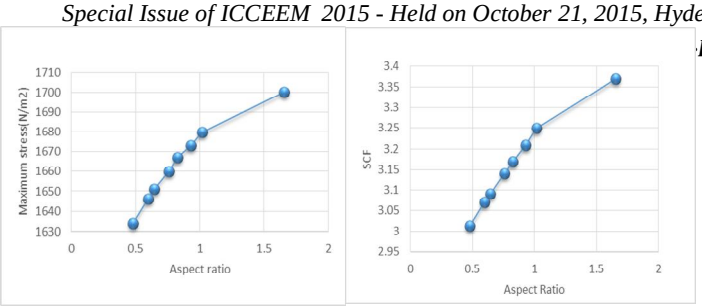


❖ For number of elements (on a particular edge) along the perpendicular direction = 10

After fixing the total number of elements depending on the computational space, the next step is to obtain the number of elements in both directions, such that aspect ratio and the stress concentration factor satisfies the required conditions. In that step these curves can help in fixing the element distribution.

Multi-Scale Simulation Results

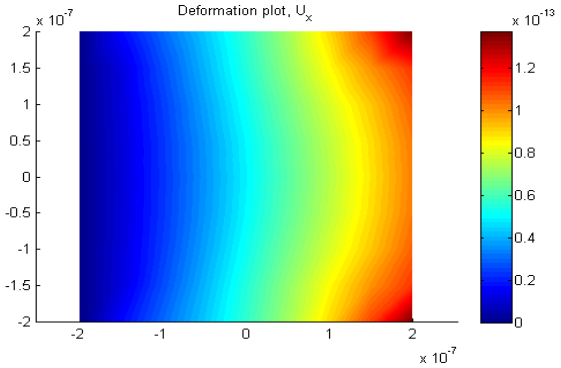
After deciding the model of coupling and with, FEM and MD tool ready, multi-scale simulation of ESCM model with periodic boundary conditions (PBC's) can be performed. From the understanding developed in the previous section we can fix the meshing and run the simulation on the coupling model specified in previous section.

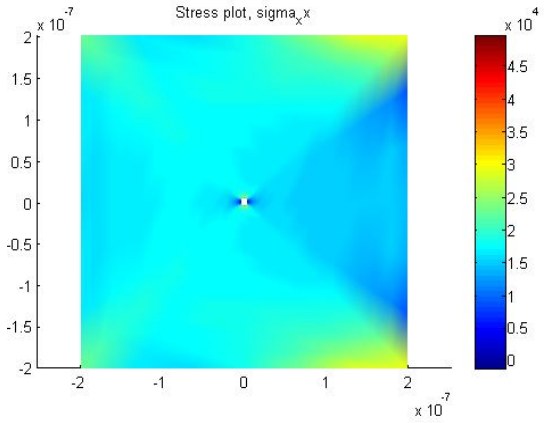
FEM analysis of model

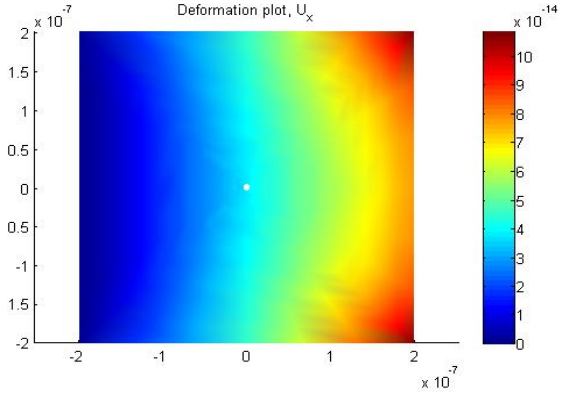
But before running the multi-scale simulation, simple FEM analysis is done for the model so as to get a rough idea about the order and magnitude of the stress and displacement distribution. The analysis is done for two cases:

- FEM analysis of the model of given dimensions (simple 2D plate)
- FEM analysis of the model without the MD domain (2D plate with a hole)

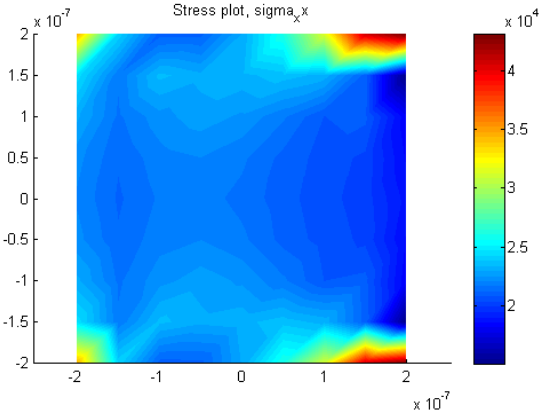
These results roughly gives the range of the stress and displacement pattern. The equilibrium values should converge somewhere between the values obtained in the above two analysis.







For case 1: Full Coupling Model



For Case 2: Coupling Model without MD domain

Meshing and Simulation result

Based on the understanding, about the mesh quality developed in the above section, the number of elements along both the perpendicular and the radial direction are fixed such that aspect ratio should be around unity and the stress concentration factor should be near to its theoretical value. The mesh finally has 18 elements along radial direction and 24 elements along circumference. The aspect ratio of the smallest, near to the interface region, is around 1.6 which is sufficiently good. The final mesh of the model with enlarged central part is shown below –

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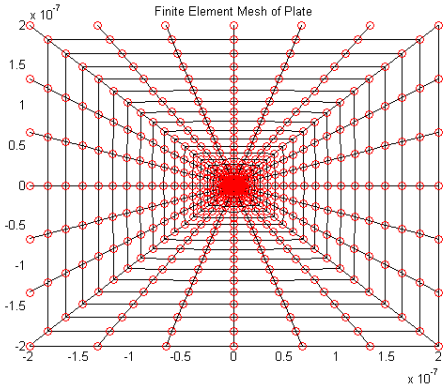
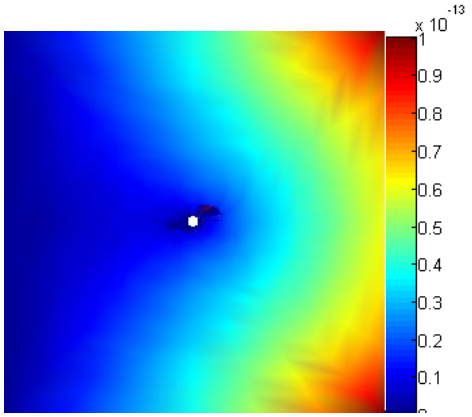
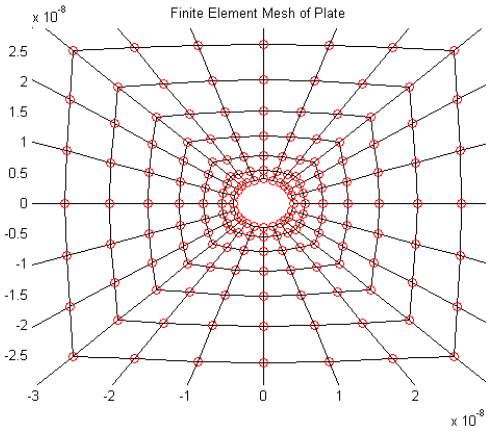
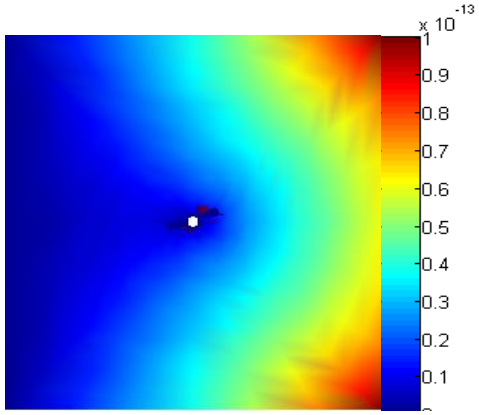


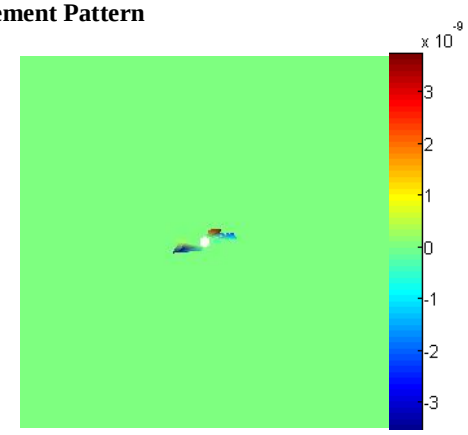


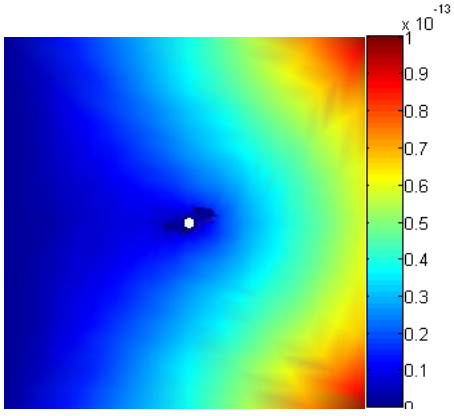




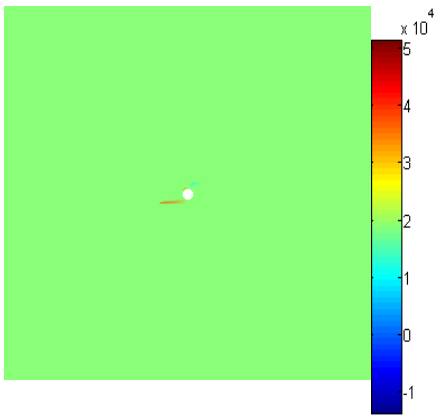
After this the simulation is run utilizing the code written in Matlab. The results obtained from the simulation are shown here.

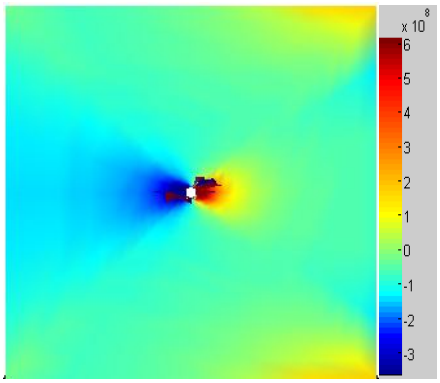
Displacement Pattern





Stress Distribution





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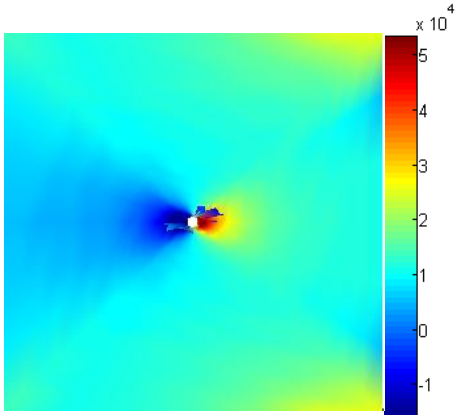
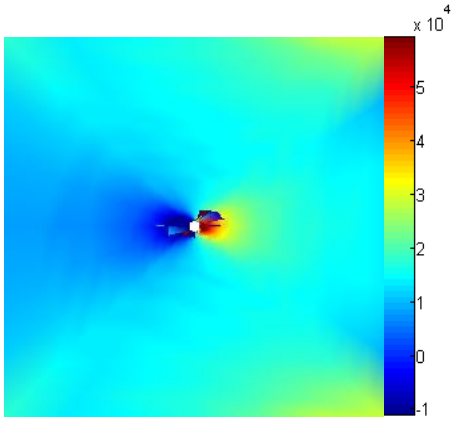
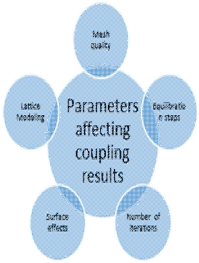




Analysis of the results

The plots of stress and displacement fields obtained above have many interesting features.

The first picture in both field is the distribution at higher scale and it is found to be uniform. Thus the order of the results obtained is same in most of the region except few very small pockets of stress or displacement concentrations. The reason for these concentration cannot be predicted at this level. Better level of maturity is required with the analysis to remove these pockets and obtain uniform and accurate distribution.



Secondly, the color pattern in both of the stress and displacement field is more closer to the plate with a hole case, which should be closer to the case of simple 2D plate. This may be due to the compromise being done in the accuracy of the analysis by using PBC's. But nothing can't be said accurately that the color pattern as the mesh used in the reference analysis is different than the one used in the multi-scale model FEM domain.

The most important thing about the results are that the time taken and complexity involved has been reduced to great deal. This is also the major objective of the present work even though it comes with certain compromise with accuracy. Another promising thing is that a state of equilibrium has been attained by the model even with some anomalies. Thus one can assume that the current approach with some modifications can give better results.

CONCLUSION

The results obtained from the modified ESCM model are exciting in terms of the opportunity they can provide for future work in the area. The level of maturity is not enough to study and further modify the model. But if certain level of maturity is achieved, it can be very really helpful in making the multi-scale methods more efficient and effective.

Although the results obtained are promising in some areas, it requires more attention and focus in some other areas also. Certain observed things cannot be explained with current level of maturity in the topic. But by utilizing the interplay of various factors affecting the simulation, one can gain experience and, identify and modify the factors so as to obtain sufficiently accurate results.

A conclusion section is not required. Although a conclusion may review the main points of the paper, do not replicate the abstract as the conclusion. A conclusion might elaborate on the importance of the work or suggest applications and extensions. There are many factors which directly or indirectly influence the coupling of MD and FEM in ESCM model. It is very important to understand the behavior of each of the factor and the manner in which it is affecting the simulation, if anybody wants to gain command over the field. Some of the most important factors are listed below. One can study the interplay of these crucial factors and come over the modifications required in the current model.

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