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A Combined X-Fem And Level Set Approach For Modeling Composite Material's Micro Structure

Himanshu Kumar

University of Texas at El Paso, kumarhimanshu305@gmail.com

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A COMBINED X-FEM AND LEVEL SET APPROACH FOR MODELING COMPOSITE
MATERIAL'S MICRO STRUCTURE

HIMANSHU KUMAR

Department of Mechanical Engineering

APPROVED:

John F. Chessa, Ph.D., Chair

Cesar Carrasco, Ph.D

Mujibur R. Khan, Ph.D

Benjamin C. Flores, Ph.D.
Acting Dean of the Graduate School

Dedicated to my Parents

A COMBINED X-FEM AND LEVEL SET APPROACH FOR MODELING COMPOSITE
MATERIAL'S MICRO STRUCTURE

By

HIMANSHU KUMAR

THESIS

Presented to the Faculty of the Graduate School of
The University of Texas at El Paso
in Partial Fulfillment
of the Requirements
for the Degree of
MASTER OF SCIENCE

Department of Mechanical Engineering
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A COMBINED X-FEM AND LEVEL SET APPROACH FOR MODELING COMPOSITE MATERIAL'S MICRO STRUCTURE

Abstract

By

Himanshu Kumar

Composite materials are usually made of fibers and binding matrix. It's always a challenge to model composite materials' microstructure through the traditional finite element method because construction of an approximation space which is discontinuous across a given line or surface will place strict restrictions on the FE mesh. The interfacing of fibers in composites' microstructure through the standard finite element method is irksome and tedious because the presence of fiber presents a discontinuity in the binding material. In this present work, the composite's microstructure is modeled through the combined approach of Level Set and Extended Finite Element Method. The fiber is modeled implicitly through level set initialized by sign distance function within the framework of XFEM where mesh edges and faces do not have to align with discontinuities (e.g. cracks, holes, interfaces, etc). In XFEM, an enrichment function is used to locally enrich the approximation space by classical Finite Element Method that enables the precise approximation of discontinuity. Theoretical background information is provided on XFEM, Level Set Method, signed distance computation and its algorithms with the description of fiber modeling technique.

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Chapter1: Introduction

Enriched Finite Element Method, often abbreviated X-FEM [1], [2], is a promising computational technique to mesh cracks, material interfaces, voids, etc. The main attractive feature of X-FEM is that it maintains the characteristics of the finite element framework, such as sparsity and symmetricity of the stiffness matrix, but implements a single-field variational principle that provides freedom to finite element mesh to not conform to internal boundaries like material interface and holes that means a single mesh is sufficient enough for modeling the crack propagation , phase change or change in material interface in two or three dimensional problem.

XFEM provides facilities to analyze structure of complex geometries since it is not necessary for mesh to match the geometry and woven fiber poses a complex shape, hence it would be good idea to model composites material's microstructure through XFEM coupled with level set data. Level set data generation process is most vital step to construct XFEM approximation because the surface of interest (discontinuity e.g. holes, material interface, cracks etc) can be easily described through zero level set and level set data is also helpful in enrichment process. Since composite materials provide improved mechanical properties and offer promising potential applications in almost every field of engineering and industry, they are receiving enormous attention in every field of material science. The development of materials modeling has experienced a huge growth in the last 10 years. Ever increasing computational power, advanced computing methods like parallel computing and multigrid technique, improved algorithms and novel mathematical formulation and concepts making simulation and modeling possible at its best by extending the computing technology [5].

This thesis is concerned with modeling of microstructure using the combined approach of level

set method and X-FEM. In this proposed microstructure, fibers within the matrix have a woven geometry impregnated by metals or other materials which are assumed to be part of the composite material's microstructure. To model this microstructure, a micro-scale representative volume element (RVE) is required. The RVE is a volume element that is statistically representative of typical material properties, including properties of the microstructure [6] such as (strength, toughness, ductility) a definition proposed by Drugan and Willis (1996) states, "*it is the smallest material volume element of the composite for which the usual spatially constant (overall modulus) macroscopic constitutive representation is sufficiently accurate model to represent mean constitutive response.*" Here an RVE is defined which explicitly models the fiber in a microstructure. It is this RVE which is then can be used to extract the macro-scale constitutive parameters for the component-level finite element model.

Using this approach, an RVE is modeled in GMSH (developed by Christophe Geuzaine and Jean Francois) after specifying input variables related to the fiber geometry. A set of GMSH-compatible subroutines is written in MATLAB to extract the nodal and element data, generate a level set, and display the mesh. The RVE is housed within a three-dimensional grid, which is assumed to consist of some matrix material. These surrounding matrix points were defined with a high number of nodes in order to evaluate the level set for the fiber which is initialized by signed distance field.

A numerical technique called Level set method has been used in this work, for surface tracking of fiber. It has been known that evolution of moving interface or discontinuous free surface suffering with extreme topological interchanges, can be tracked or captured through computational technique named "*The Fast Marching Method*" and "*Level Set Method*" developed by Sethian and Osher [7]. Since then , significant development of these method has been done and applied to various problems associated with computer vision, robotics, material modeling, seismic analysis, fluid mechanics, tumor modeling etc;

a recent summary can be found in Sethian[8]. Burchard et al. [9] and Osher et al. [10] have considered the evolution of curves with level sets. A wide range of applications are presented in [7, 8] as well as in recent published book by Osher and Fedkiw [11] and Sethian [12].

Before building the presented composite material's microstructure modeling in this work, we first review some essential background information in material science on matrix composites, Enriched Finite element Method; Level set Method, partition of unity method etc in the following sections.

1.1Composite material:

In today's advanced society we have heavy dependencies on composite materials. Composite materials are made up of two or more distinct materials that when combined are better (stronger, tougher, and more durable) than each would be separately. For instance fiberglass was the first composite that was developed in late 1940s and still one of the most commonly used for making boat hulls, surfboards, sporting goods, swimming pool linings, building panels and car bodies [14]. We also have composites that exist in nature. For example piece of wood is a composite, with long fibers of cellulose (a very complex form of starch) held together by a much weaker substance called lignin. Cellulose is also found in cotton and linen, but it is the binding power of the lignin that makes a piece of timber much stronger than a bundle of cotton fibers.

Based on their matrix phase characteristics, composites can be generally classified into several types: *Ceramic Matrix Composites* (CMCs), *Metal matrix composite* (MMCs), and *Polymer Matrix Composites* (PMC) [35], *Carbon –Carbon composites*, *Reinforced Concrete etc.*

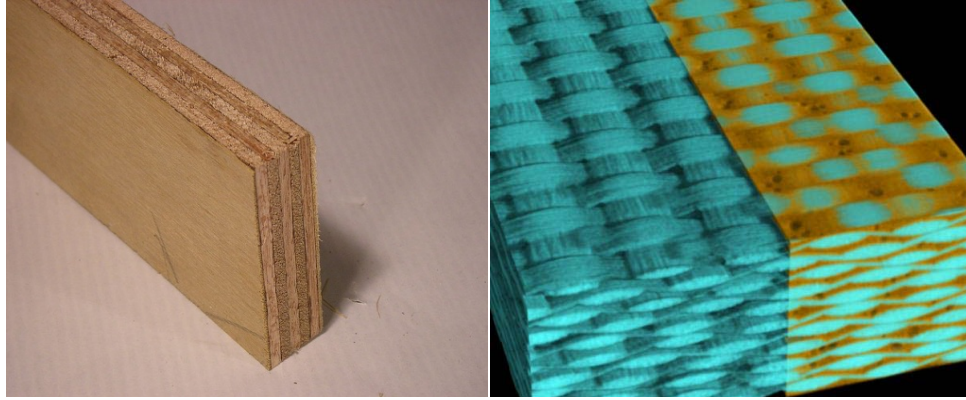


Figure 1: Composite materials: Plywood is common composite material and Glass Fiber composite material

Currently composite materials refers to materials having strong fiber that could be continuous and non continuous surrounded by weaker matrix material [13]

1.1.1Fiber and Matrix

The bonding between fibers and matrix is created during the manufacturing phase of the composite material. This has fundamental influence on the mechanical properties of the composite material.

Fibers are made of thousand of filaments and each filament usually have diameter between 5 to 15 micrometers. It's always desirable to have smallest diameter possible to enhance the rapture strength. Some of the major fiber materials are glass and Kevlar (Aramid). Glass –ceramics materials shares numerous properties of glass and ceramics. Glass-ceramics prepared by controlled nucleation and crystallization of glasses can be used in extensively different applications depending on their microstructure, mechanical, physical and chemical properties.

These properties are changeable that depends on heat treatment [15] conditions and composition of constituents in order to produce glass-ceramics of specific properties. Different verities of glass ceramic have been developed for biomedical and dental applications.



Fig 2: Cooking Top made of Glass-ceramic

Carbon fiber is some of the most popular and broadly used fiber to make composite material. Like Boron; carbon fibers also have high modulus and strength and also because of electric behavior of carbon fiber reinforced cement is relevant to the use of this material for strain sensing which is important for

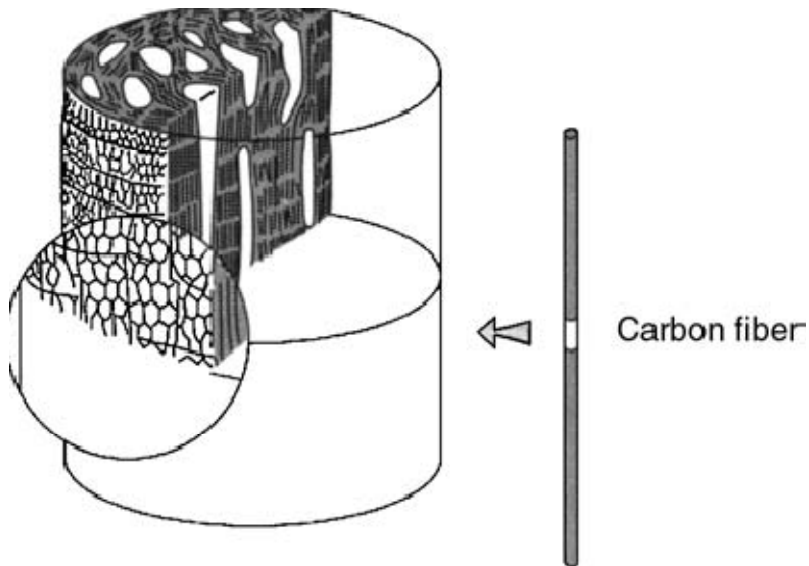


Figure 3: Structure of Carbon Fiber

smart structures, highway traffic monitoring, weighing of vehicles in motion, and structural vibration

control. The addition of short carbon fibers to cement decreases the electrical resistivity, due to the high conductivity of the carbon fibers compared to cement. The decrease occurs even when the fibers are at a volume fraction below the percolation threshold and because the cement matrix is slightly conducting. Short fibers rather than continuous fibers are preferred for concretes because of the desire for low cost and feasibility of incorporation of the fibers in a concrete mix. A low volume fraction of fibers is preferred because of the importance of low cost, good workability and high compressive strength (low air void content). [16]. Silicon carbide is used in high temperature application.

1.1.2 Relative Importance of Different Fibers in Applications

Fig --- allows one to judge the relative importance in terms of the amount of fibers used in the fabrication of composites. It can be observed that industrial demand for fiber glass is high, so produced in large scale for high performance components carbon and Kevlar fibers are widely used.

Glass fiber is constituted with silcon+sodium carbonate and calcium and its filament can be produced by pulling through small orifice of platinum plate over $1000^{\circ}C$.Kevlar fibers are yellowish in color usually made by DuPont de Neumours (USA). Kevlars are aromatic polyamides obtained by synthesis process at $10^{\circ}C$.They often poses high modulus of elasticity. Carbon fibers are obtained from petroleum product's residue and then oxidized at high temperature of $300^{\circ} C$ and then heating in nitrogen atmosphere with $1500^{\circ}C$.

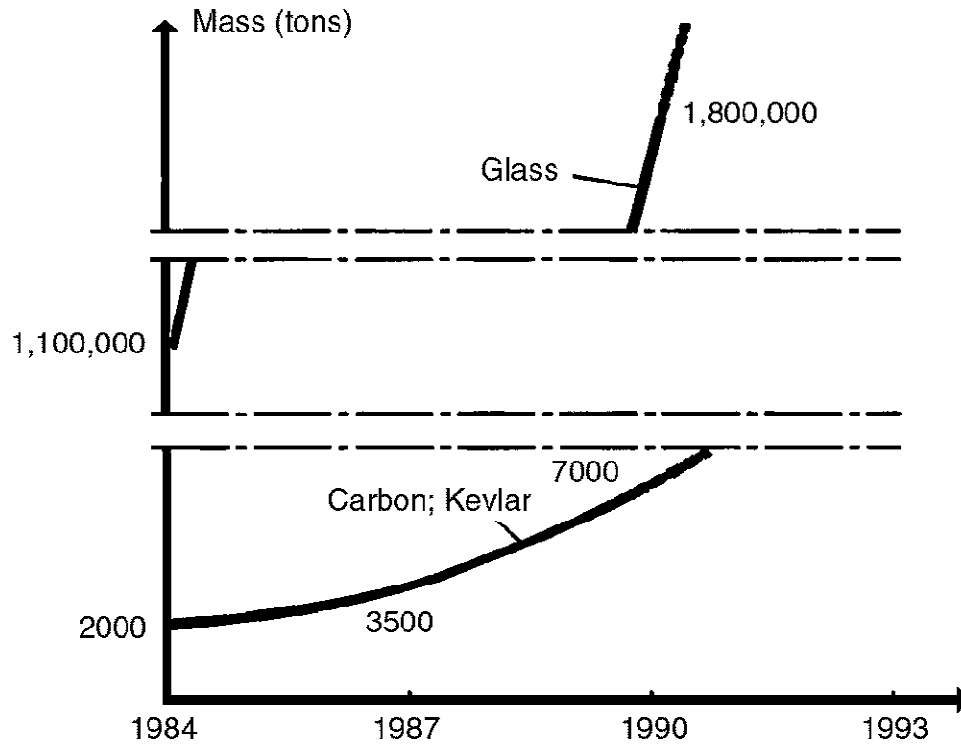


Figure 4: Relative sale volume of different fiber

Boron fibers come with 100 μm and it is obtained after reacting boron chloride and hydrogen at 1200°C. Silicon carbide's fabrication principle is very similar to the boron fiber. It is obtained through chemical vapor deposition of methyl trichlorosilane mixed with hydrogen at 1200 degree C.

As seen in Table 1¹, the fibers used in modern composites have strengths and stiffness far above those of traditional bulk materials. The high strengths of the glass fibers are due to processing that avoids the internal or surface flaws which normally weaken glass, and the strength and stiffness of the polymeric aramid fiber is a consequence of the nearly perfect alignment of the molecular chains with the fiber axis.

Table 1: Properties of Composite Reinforcing Fibers.

Material	E (GPa)	σ_b (GPa)	ϵ_b (%)	ρ (Mg/m ³)	E/ρ (MJ/kg)	σ_b/ρ (MJ/kg)	cost (\$/kg)
E-glass	72.4	2.4	2.6	2.54	28.5	0.95	1.1
S-glass	85.5	4.5	2.0	2.49	34.3	1.8	22–33
aramid	124	3.6	2.3	1.45	86	2.5	22–33
boron	400	3.5	1.0	2.45	163	1.43	330–440
HS graphite	253	4.5	1.1	1.80	140	2.5	66–110
HM graphite	520	2.4	0.6	1.85	281	1.3	220–660

1 F.P. Gerstle, "Composites," Encyclopedia of Polymer Science and Engineering, Wiley, New York, 1991. Here E is Young's modulus, σ_b is breaking stress, ϵ_b is breaking strain, and ρ is density.

1.1.3 Matrix Materials

The matrix material can be categorized in following: *Polymeric matrix*, *Mineral Matrix* and *Metallic matrix*. Thermoplastic resins like polypropylene, polyphenylene, sulfone, polyamide etc and thermoset resins that include polyester, phenolics, melamines, and silicones are an example of Polymeric matrix. Silicon carbide and carbon falls under mineral matrix that gives excellent performance under high temperature application. Aluminum and Titanium alloys are an example of metallic matrix.

1.1.4 Microstructure

The structure of prepared surfaces or thin foils observable within 25X magnification is known as microstructure. The physical properties such as strength, toughness, ductility, corrosion resistance, hardness, high-low temperature behavior, wear resistance etc decides the purpose of any material for its industrial use and those physical properties can be influenced significantly through manipulation of microstructure

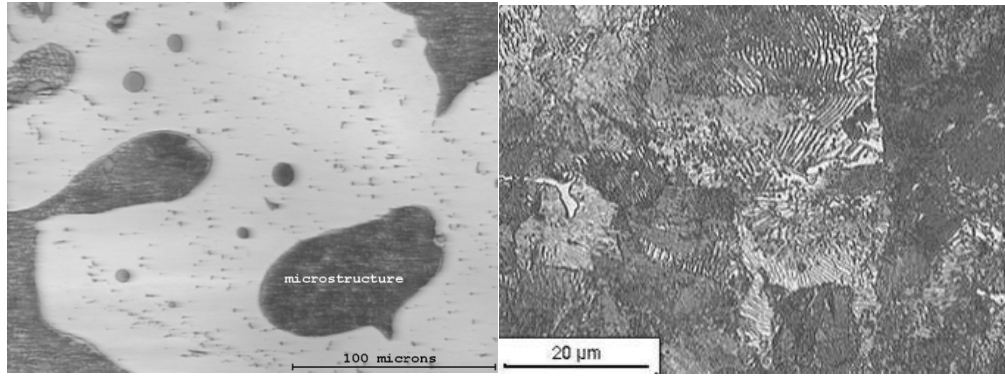


Fig 5:Microstructure (a) Al-Si microstructure (b): High Carbon steel microstructure

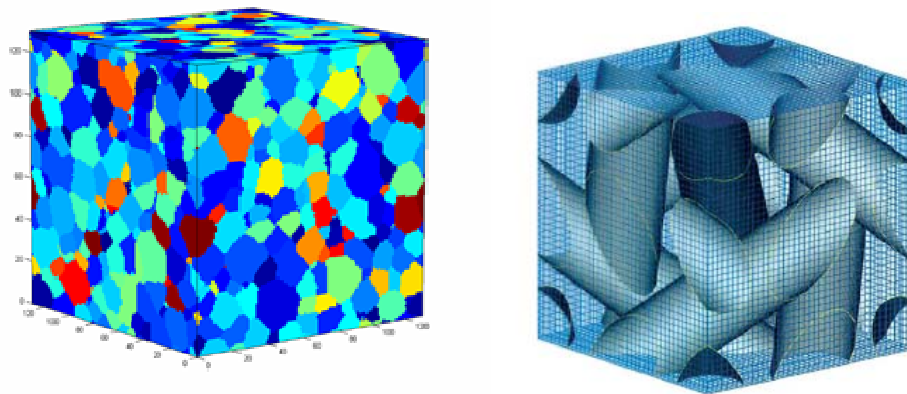


Fig 6: (a) Digital 3D polycrystalline microstructure [cmu] (b) Composite RVE using XFEM [Global Engineering & materials inc]

1.2 Modeling Technique

1.2.1 Finite Element Modeling

To studying equations on randomly shaped domains in continuum, the finite element method has been a robust numerical technique. An arbitrary domain is meshed with a collection of elements that each has some kind of spatial variation associated with them. These elements are connected at points called nodes

and the solutions to the differential equations governing the behavior of some dependent variable are obtained in an averaged sense at the nodes through the finite element approximation.

Usually variational statement of problem, that mean a weak formulation of governing differential equations is required to derive finite element method. A matrix equation that represents variation in field quantity along with other suitable method is used to discretize the weak form. These equations are then solved for matrix inversion and utilize sparsity and topology of matrix through appropriate numerical algorithms.

1.2.2 Extended Finite Element Modeling

The extended finite element method is an extension of the traditional finite element method and a very popular method for micro structural design [3][17] which works by including one or more enrichment functions to the traditional finite element approximation and invoking the partition of unity principle [18]. Solution space of standard finite element is expanded through enrichment process to enhance the accuracy of approximation enough to tackle jump or singularities in field variable that could be unresolved otherwise. Enriched function selection depends on *a priori* solution of the problem. Minimal or no remeshing in the crack propagation problem is viewed as an advantages of this method and same features makes it attractive for simulation of complex microstructure ,especially at interface and for prognostic modeling [19].

1.3 Numerical Methods for tracking static or moving interface

1.3.1 Level Set Method

Level set method (LSM) is a widely known tool for tracking interface. Many XFEM formulations take advantages of the level set method. This approach was introduced by Osher and Sethian that says the idea of making the surface from the original curve instead of following of interface itself. In LSM, the interface of interest is represented as the zero level set of function $\phi(\mathbf{x})$. This function is a dimension

higher than the dimension of the interface. Several benefits of level set tracking scheme is realized .It computes the motion of interface on Eulerian mesh instead of Lagrangian mesh and method can be implemented on higher dimension problems. Using level set function $\phi(x)$, geometric properties of interface can be acquired. Requirement of higher dimension function by level set leads to higher storage and computational cost that shows the method's drawback.

1.3.2 Fast Marching Method

FMM was initially formulated by Sethian in 1996 and later improved by Sethian himself in 1999 and Chopp (2001).In order to track moving hypersurface, Fast marching method (FMM) finds the first arrival point, the interface passes. This method works best on problems in which sign never changed by its speed function and it signifies that either front is progressing forward or backward.FMM tolerates discrepancies in speed but expecting direction to be unidirectional. The problems transformed to stationary formulation because of FMM behavior, mentioned above and eventually reduced the computing time significantly as compared to level set method.

1.3.3 Ordered upwind Method

As we know that in FMM solution is updated thoroughly from known values to unknown marks. This based on actuality that information should always come from the direction of the gradients of the front. However, this is not true when speed varies and other factors affects like irregularity in direction, then one can't assume that information always come at trajectory perpendicular to the evolving wave front. So to follow the characteristics direction, a solution is proposed in which the ratio between the fastest and slowest speed at each point is defined. This method is called the ordered upwind method (OUM). This maintains the procedure of point ordering while systematically computing the solution by relying on previously known computed information. [19]

1.4 Outline of thesis

The outline of this thesis is as follows. In the next section a brief introduction of level set method and signed distance function is given and in chapter 4, XFEM is introduced .In chapter 5 modeling methodology of fiber and matrix is addressed that includes the discussion of computer code and computing concepts of shortest distance. Literature review is presented in chapter 2. Conclusion and future works is given in chapter 6 where coupling of level set data with XFEM is discussed.

Chapter 2: Literature Review

Thomas Hettich and Ekkehard [20] discussed in his paper to model interface material failure through combined approach of extended finite element method and level set method . In this literature they defined material layout by level set functions. The interface is modeled mathematically as a zero level set of smooth function $\varphi: R^d \rightarrow R$ where spatial dimension of the given problem $\Gamma=\Gamma(t)= \{x \in R^d | \varphi(x, t)=0\}$ where it can be observed that Γ can be defined as the set of points x in R^d that make the isocontour $\varphi=0$ of implicit function φ . In this case the material's layout of solid phase contains circular inclusion that is encompassed with matrix. The paper explained that interface is not moving so the initial conditions $\varphi(x, 0)$ is same for all time, which is used to introduce level set function as a signed distance function. For this case

$$\varphi(x) = \varphi(x, 0) = \min \{ ||X - X_{in,i}|| - r_{in,i} \} \quad \text{for } i = 1, \dots, n_{in} .$$

is the signed distance function which means the shortest distance from the point x to the interface as well as the material phase in which the point is located are known.

Ventura et al [21] talked about a vector level set method to model propagating cracks where nodal data is used to describe the crack trajectory instead of geometrical entities. He claimed that solving partial differential equation is not necessary to be solved to update level set data. As the crack grows the nodal description is getting updated through geometrical operation on data whereas in classical in level set method, a evolution equation has to be solved. In his paper he presented this novel approach to two dimensional applications that can be easily implemented on three dimensional cases where crack's evolution as well as it geometrical description is more complex.

Chessa et al.[22] used signed distance function to represent the interface that separates the solid and fluid region of its domain .In this case the interface between fluid region and solid region is moving ,hence level set update is an vital task that has to be performed frequently .The signed distance is basically updated by level set method with the idea that total time derivative of level set function which moves with the interface should set to zero that basically enforcing a condition on level set function to remains constant on interface. The complete update algorithm is given in Chessa et al.

Sukumar et al [17] discussed about the methodology to model arbitrary holes and inclusions .The level set method is used to represent the holes' location and material interface whereas level set function is used to develop the local enrichment for material interface. Sukumar and his colleagues introduced a different level set function for circular voids as

$$\varphi(\mathbf{x}, 0) = \min_{\substack{\mathbf{x}_c^i \in \Omega_c^i \\ i=1,2,\dots,n_c}} \{ \|\mathbf{x} - \mathbf{x}_c^i\| - r_c^i \}.$$

where Ω_c^i is the domain of the i th void , n_c is the number of circular voids, and \mathbf{x}_c^i and r_c^i are the center and the radius of i th void, respectively.

N. Moes et al [23] discussed about the methodology to solve microstructure with complicated geometries by using XFEM.

M Kastner et al [24] worked on multi-scale simulation of fiber-reinforced polymers and discussed an automated XFEM-modeling procedure of RVE.

Colin B. Macdonald and Steven J. Ruuth [25] used closest point method which is technique for solving partial differential equations (PDEs) on surface .In this paper author introduced a weighted Essentially Non-Oscillatory (WENO) interpolation step into the closest point

Chapter 3: Interface Tracking Technique: Level Set Method

3.1 Level Set Method

Level set methods have become widely used for capturing interface evolution especially when the interface undergoes through severe topological changes, such as “merging or pinching off”. [26]. Level Set Method exploits the Eulerian partial differential equation standpoint instead of using geometric Lagrangian perspective to treat boundary motion. This provides a robust numerical approach for interface analysis and related computation that is expected to show corners and face extreme topological changes as they evolve. The evolution can be described through partial differential equation in function that defines the surface, hence implicit representation of surface is possible. Hyperbolic conservation law is prominent in stabilizing the numerical solution to partial differential equation. [27].

In Level Set Formulation of moving fronts (or active contours), the fronts, denoted by C , are represented by the zero level set $c(t)=\{(x, y)| \phi(t, x, y)=0\}$ of a level set function $\phi(t, x, y)$. The evolution equation of the level set function ϕ can be written in the following general form:

$$\frac{\partial \phi}{\partial t} + F |\nabla \phi| = 0$$

which is also called the *level set equation* [11]. The function F is a scalar velocity field or called as a speed function [28] defined as

$$F = \mathbf{n} \cdot \mathbf{v} = \frac{\nabla \phi}{|\nabla \phi|} \cdot \mathbf{v}$$

So as we know, LSM is a numerical technique to track moving interfaces that is based upon the idea of representing the interface as a level set curve of a higher dimensional function $\phi(\mathbf{x}, t)$

3.1.1 Level Set Illustration

The first primary objective is to define a signed distance function ϕ to the hypersurface (or interface) within the computational domain so the free surface doesn't need to be explicitly tracked. The concept of Level set implementation could be easily understood through illustration explained below.

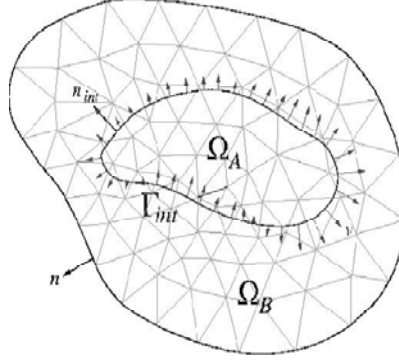


Figure 7: A domain divided into two regions A and B

Consider the domain Ω as shown in figure ... that is composed of two different regions A and B respectively denoted by Ω_A and Ω_B . The interface between the region A and B are shown by Γ_{int} moving with vector velocity field \mathbf{v} . The outward normal to interface is denoted n_{int} .

The distance function can be defined as

$$d(x, t) = \min_{z \in \Gamma_{int}} (|x - z|)$$

where z is an element of Γ_{int} .

The definition of Level set can be summarized as follows

$$\Phi(x, t) = \begin{cases} d(x, t) & \text{on } \Omega_B \\ -d(x, t) & \text{on } \Omega_A \\ 0 & \text{on } \Gamma_{int} \end{cases}$$

3.1.2 Mathematical Derivation

Here we briefly explain how the level set equation is formulated. See [29] for more details and applications of level set method.

Assume $\Gamma(t=0)$ is a closed $(N-1)$ -dimensional hypersurface (or interface), which is moving with speed F on its normal direction. The level set equation is an Eulerian formulation for the motion of the hypersurface $\Gamma(t)$. It is based on the idea of embedding the propagating hypersurface as the zero level set of a higher dimensional function $\phi: R^n \rightarrow R$. Define

$$\Phi(x; t=0) = \pm d$$

where d is the signed distance function from initial hypersurface $\Gamma(t=0)$. Then in

$$\Gamma(t=0) = \{x \mid \phi(x, t=0) = 0\}$$

order to produce an equation for $\phi(x; t)$ so that the moving hypersurface at time t , $\Gamma(t)$, is always the zero level set of $\phi(x; t)$: $\Gamma(t) = \{x \mid \phi(x; t) = 0\}$ for all t , let $x(t)$ be the path of a point on the evolving hypersurface, then $xt \cdot n = F(x(t))$ where n is the normal direction of the hypersurface at point $x(t)$. Zero level set of ϕ always matching the evolving hypersurface Γ means that

$$\phi(x(t); t) = 0$$

Take derivative with respect to t :

$$\nabla\phi(x(t), t) \cdot x'(t) + \phi_t = 0$$

From $xt \cdot n = F(x(t))$ and $n = \frac{\nabla\phi}{|\nabla\phi|}$; we have

$$\phi_t + F|\nabla\phi| = 0$$

And this is the level set equation for hypersurface (interface) propagating at speed F on normal direction.[30]

3.2 Signed Distance Function

The distance d from a point x to an interface Γ is defined as,

$$d = \|x - x_\Gamma\|$$

where x_Γ is the normal projection of x on Γ in figure below. The signed distance function can be defined as ,

$$\phi(x) = \pm \min_{x_\Gamma \in \Gamma} \|x - x_\Gamma\|, \quad \forall x \in \Omega,$$

Where the sign is different on the two side of discontinuity and $\|\cdot\|$ denotes the Euclidian norms that can be defined as

$$\|x\| = \sqrt{x_1^2 + x_2^2 + \dots + x_n^2}$$

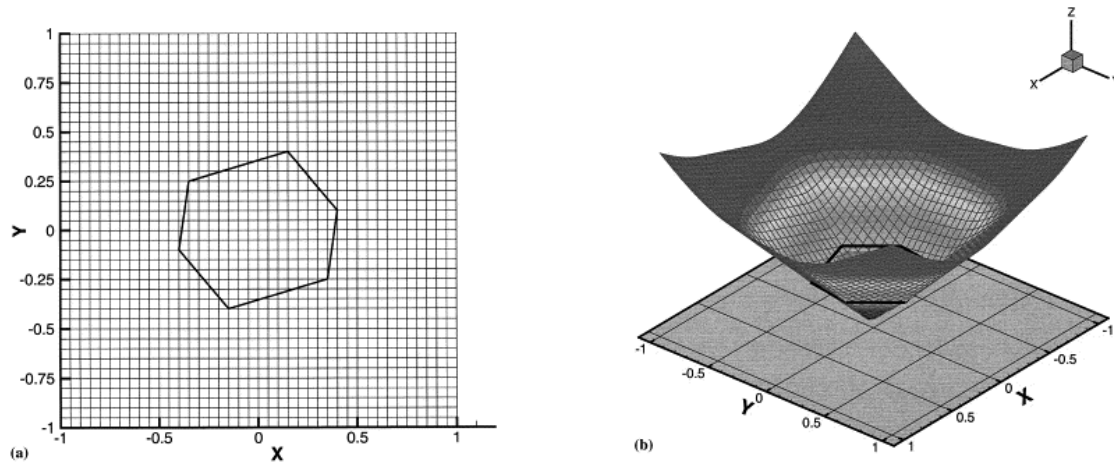


Figure 8: Level set function for hexagonal interface: (a) Mesh; (b) Level Set function taken from N Sukumar

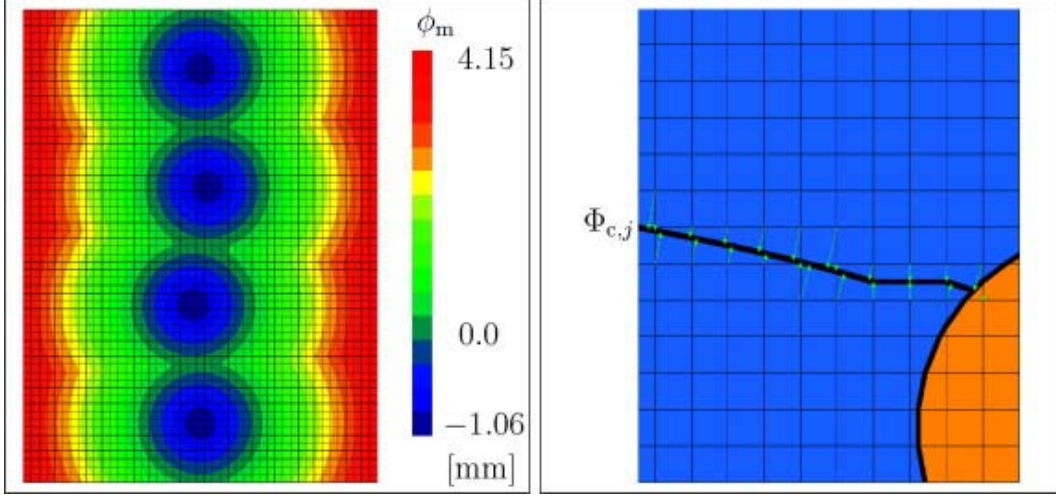


Figure 9: Level set representation of composite and matrix crack

3.3 Other Types of Level set

The signed distance function is perhaps the most preferred type of level set function. However, there are other types, such as circular, elliptical and polygonal functions. The circular level set functions can be defined as (Sukumar et al. 2001)

$$\varphi_{,i}(\mathbf{x}) = \min_{\substack{\mathbf{x}_c^j \in \Omega^j \\ j=1, \dots, n_c}} \{ \|\mathbf{x}_i - \mathbf{x}_c^j\| - r_c^j \}$$

where Ω^j is the domain of j th void, number of circular holes are denoted by n_c and location of the centre of the j th hole with radius r_c^j is given by \mathbf{x}_c^j .

Sukumar et al. [17] also defined the elliptical level set function as follows

$$\varphi_i(\mathbf{x}) = \min_{j=1, \dots, n_c} \{ f(\xi^j) \}$$

where $f(\xi^j)$ denotes the equation of ellipse j in the local coordinate system,

$$f(\xi^j) = \|\xi^j\| - 1$$

and

$$\xi^j = \left(\frac{\bar{x}^j}{a_j}, \frac{\bar{y}^j}{b_j} \right)$$

where a_j, b_j are the semi-major and semi-minor axes of ellipse with centre x_c^j where

$$\bar{\mathbf{x}}^j = R^j(\mathbf{x}_i - \mathbf{x}_c^j)$$

Polygon level set function according to Sukumar et al [17]

$$\phi_i(\mathbf{x}) = \|\mathbf{x}_i - \mathbf{x}_{\min}\| \text{sign}[\mathbf{n}_{\min} \cdot (\mathbf{x}_i - \mathbf{x}_{\min})]$$

$$\|\mathbf{x}_i - \mathbf{x}_{\min}\| - \min_{\substack{\mathbf{x}_j \in \Gamma_j \\ j=1, \dots, p}} \|\mathbf{x}_i - \mathbf{x}_j\|$$

whereas \mathbf{x}_{\min} is the orthogonal projection of \mathbf{x} on interface Γ and \mathbf{n}_{\min} is the normal to the interface at \mathbf{x}_{\min} . If there is no unique normal at \mathbf{x}_{\min} then sign is positive and if $\|\mathbf{x}_i - \mathbf{x}_{\min}\|$ belongs to the cone of normal at \mathbf{x}_{\min} then sign is negative.

Chapter 4: Extended Finite Element Method –A Minimum Remeshing Technique

The extended finite element method (XFEM) is a numerical method that enables a local enrichment of approximation spaces. The enrichment is performed through the partition of unity concept. The method is useful for the approximation of solutions with prominent non-smooth characteristics in small parts of the computational domain, for example near discontinuities and singularities. In these cases, standard numerical methods such as the Finite element method or Finite Volume method often exhibit poor accuracy. The XFEM offers significant advantages by enabling optimal convergence rates for these applications.[31]

4.1 Non-smooth solution properties: Discontinuities and singularities

An abrupt change in any field quantity over a length which is negligible compared to the range may be defined as a discontinuity. In solids, the presence of holes, cracks and inclusions on material interface are known as discontinuities. Pressure and velocity field may pose discontinuities on the interface of two fluids. However discontinuities can be categorized into two different types: Weak and strong discontinuities.

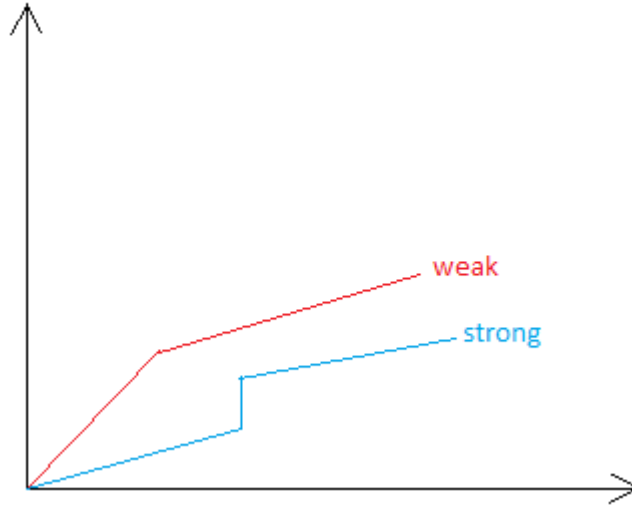


Figure 10: (a) Weak discontinuities (b) Strong discontinuities

The above figure explains the nature of both types of discontinuities. We can see that for weak discontinuities, the field quantity experiences a change in the gradient (kink) whereas strong discontinuities' field quantities have simply jumped. The other kind of non-smooth solution that is frequently encountered is the *singularity*, which often occurs at the crack tip. The phenomenon of oscillation in wave propagation also falls into the category of non-smooth solution. Special care is required for the mesh generation during the approximation of non-smooth solution through standard numerical methods like FEM or the Finite Volume Method in which the element edges must align to the discontinuities and mesh refinement is required near singularities. In contrast, the XFEM is able to achieve optimal convergence rates on structured meshes where arbitrary discontinuities and singularities are present in element interiors.[31]

In XFEM these discontinuities are described through scalar level set functions, constructed on the domain and a function's zero level set represents the interface or discontinuity. For example, in the figure below a domain is subdivided into two sub domains named A and B on the both

side of the discontinuity having circular geometry with radius r around $(0, 0)$ on structured mesh. A sign convention for level set is as follows: negative for region A and positive for region B.

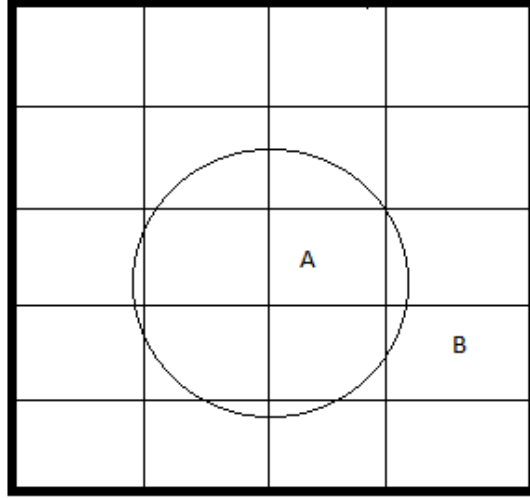


Figure 11: A circular interface plotted on structured mesh

Now in this two-dimensional case, the discontinuity can be defined by the level set function

$$\phi(x, y) = \sqrt{x^2 + y^2} - r \quad (4.1)$$

which is zero on the circle. The level set function is naturally defined by discrete values at $\phi_i = \phi(\mathbf{x}_i)$ and they can be interpolated in the element interior by the standard finite element shape function

$$\phi^h(\mathbf{x}) = \sum_{i \in I} N_i(\mathbf{x}) \cdot \phi_i \quad (4.2)$$

4.2 Basics of FEM: Isoparametric finite elements, a short review

Consider a domain in the state of equilibrium discretized by four node quadrilateral finite element mesh,

as shown in fig 12. According to the finite element methodology the coordinate $\mathbf{X}^T = (x, y)$ are interpolated from the nodal value $\bar{\mathbf{X}}^T = (x, y)$

$$\mathbf{X} = \sum_{j=1}^4 N_j \bar{\mathbf{X}}_j \quad (4.3)$$

where N_j is the matrix of finite element shape function.

$$N_j = \begin{bmatrix} N_j & \mathbf{0} \\ \mathbf{0} & N_j \end{bmatrix} \quad (4.4)$$

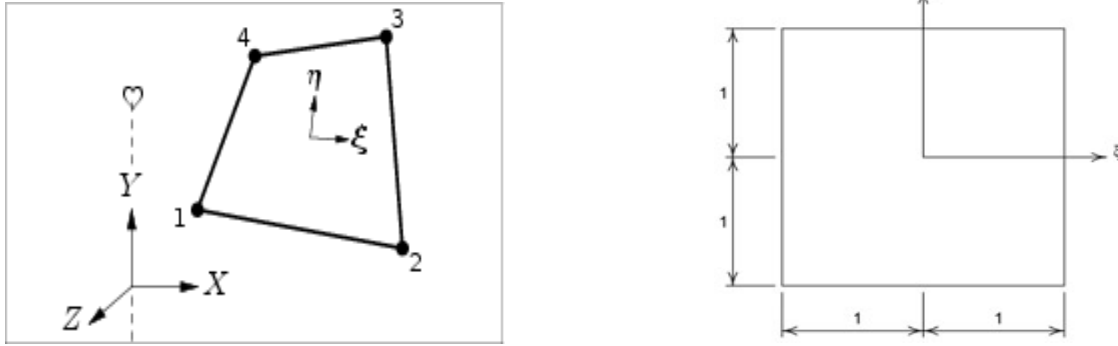


Fig 12: An Isoparametric finite element

In an Isoparametric finite element representation, displacement field $\mathbf{u}^T = (\bar{u}_x, \bar{u}_y)$ are similarly interpolated from the nodal displacement nodal value $\bar{\mathbf{u}}^T = (\bar{u}_x, \bar{u}_y)$.

$$\mathbf{u} = \sum_{j=1}^4 N_j \bar{\mathbf{u}}_j \quad (4.5)$$

The strain field is computed directly from equation

$$\boldsymbol{\varepsilon} = \sum_{j=1}^4 B_j \bar{\mathbf{u}}_j \quad (4.6)$$

where the matrix B_j is defined in terms of derivative of the shape function N_j ,

$$B_j = \begin{bmatrix} \partial N_j / \partial x & 0 \\ 0 & \partial N_j / \partial y \end{bmatrix} \quad (4.7)$$

where chain rule is evoked to determine the coefficient of B_j :

$$\begin{Bmatrix} \partial N / \partial x \\ \partial N / \partial y \end{Bmatrix} = J^{-1} \begin{Bmatrix} \partial N / \partial \xi \\ \partial N / \partial \eta \end{Bmatrix} \quad (4.8)$$

where J is the Jacobian matrix

$$J = \begin{bmatrix} \partial x / \partial \xi & \partial y / \partial \xi \\ \partial x / \partial \eta & \partial y / \partial \eta \end{bmatrix} \quad J^{-1} = 1 / \det J \begin{bmatrix} \partial y / \partial \eta & \partial y / \partial \xi \\ -\partial x / \partial \eta & \partial x / \partial \xi \end{bmatrix} \quad (4.9)$$

Finally, the stiffness matrix K_e of an element Ω_e can be determined form :

$$K_e = \int_{\Omega_e} B^T D B \, d\Omega \quad (4.10)$$

where D is the material stress-strain or constitutive matrix [19]

4.3 Partition of Unity

Like Hp cloud, Generalized Finite Element Method (GFEM) and other mesh free method, Extended Finite Element Method (XFEM) also comes under the class of Partition of Unity method. This method has been constantly using for replicating various science and engineering problems. As we know, that in finite element, shape function N_I is associated with node I in a mesh. Let $\omega_I = \{x: N(x) > 0\}$ be a region of influence for N_I . The nodes related to the element are given by the connectivity of the element and ω_I is the collection of the elements that are associated with specific node I [32].

The partition of unity approximation for a scalar-valued function u can be written in general form

$$u^h(\mathbf{x}) = \sum_{I=1}^N N_I(\mathbf{x}) \left(\sum_{\alpha=1}^M \psi_{\alpha}(\mathbf{x}) a_I^{\alpha} \right) \quad (4.11)$$

Where ψ_{α} are enrichment functions, and \mathbf{a}_I^{α} are unknown coefficients that are related with node I , the enrichment function ψ_{α} and a specific geometric entity. The finite element shape functions create a partition of unity as $\sum_I N_I(\mathbf{x}) = 1$. From above equation (4.11), we can observe that traditional finite element space ($\psi_I = 1$; $\psi_{\alpha} = 0$; ($\alpha \neq 1$)) is a sub-space of the product $N_I \alpha$ has compact support. A standard Galerkin procedure is used to obtain the discrete equations, and the symmetry and sparsity of the stiffness matrix are also retained. Some important properties that makes PUM a powerful tool for local enrichment procedure within finite element method are following given by N Sukumar et al[32]

1. point, line singularities and surface discontinuities can be handled without the need of discontinuous surface to be aligned with the finite element mesh.
2. automatic enforcement of continuity.
3. Can include application-specific basis function to better approximate the solution.

4.4 Enriched Finite Element Method (XFEM)

The purpose of enriched finite element (XFEM) is to enlarge the approximation space of standard finite element so it can include the solution space. The enrichment of standard finite element basis enhanced the convergence that is noteworthy. (Melenk and Babuska 1996) introduced partition of unity and with this approach the enrichment scheme has been improved a lot. The process of constructing enriched approximation is explained below

In XFEM the standard finite element approximation

$$u^h(x) = \sum_{I \in N} N_I(x) u_I(t) \quad (4.12)$$

is enriched with function $\psi(x, t)$ as follows

$$u^h(x) = \sum_{I \in N} N_I(x) u_I(t) + \sum_{J \in N^{enr}} N_J(x) \psi(x, t) a_J(t) \quad (4.13)$$

where N is a set of node number in discretization and N^{enr} is a set of enriched nodes. It can be observed that if value of $a_J = 1$ and $u_I = 0$, then function ψ can be recovered. This enables finite element approximation to reproduce a general function ψ . As we can see the N^{enr} is a subset of total node in discretization. By only enriching in region where enrichment is required, the additional computational effort is kept minimal. It is easy to implement this method in any standard finite element code. Enriched approximation contains the standard finite element approximation, so the enrichment can only provide better accuracy over standard finite elements. The error can never be greater than that of standard finite element method.

Chapter 5: Modeling Methodology and Zero Level Set Computation

5.1 Modeling Methodology Overview

The proposed composite material's microstructure has woven shaped fiber infused in the composite's matrix material and forms REV that can be consider as homogenize two phase basic cells. Level set technique is used for the material interface description that separates the two phase. Level set technique within the framework of XFEM is a sound approach to describe a jump in strain field within the element cut by any material interface. The idea of work can be given through example given below with woven cell taken from [23] for illustration purpose. The example is based on the numerical experiment done in [34].The geometry of the unit cell is shown in figure 12.The finite element mesh developed in J.M Guendes, N.Kikuchi [34] is shown in figure 13

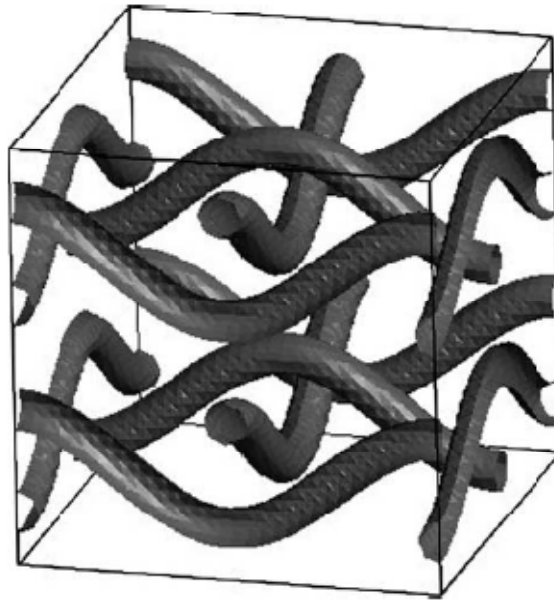


Figure 13: Woven cell geometry

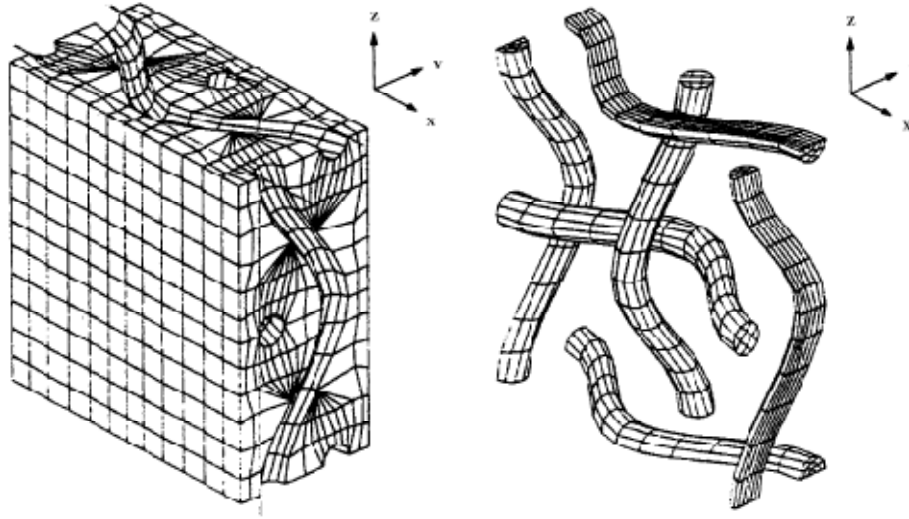


Figure 14: Mesh constructed in the paper by Kikuchi and Guedes for FEM analysis

In figure 12 the fibers are arranged in woven shape and completely confined in cell which is treated as a matrix. The cubical cell shown in figure is meshed uniformly with structured mesh that will help in further XFEM computation is shown in figure in next section.

In [24] author explained the procedure for automated modeling procedure of local material in RVE in which he converts three dimensional fiber's geometric arrangement in RVE in to numerical XFEM model that can be easily explained through figure 14 in which an idealized geometric model of three dimensional local material structure is shown.

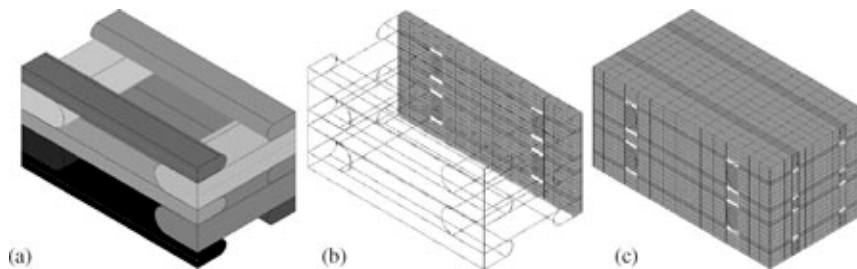


Figure 15: Automated XFEM-modeling of RVE procedure from the paper M Kastner and colleagues

Figure 14(a) shows a 3D geometric modeling that is the genesis of Kanstner's modeling procedure where fibers n_f in RVE is represented by volume v_f in this geometric model that excludes the surrounding matrix material. In later step, layers of volume is superimposed on the fiber model as shown in figure 14(b) to completely fill the cuboids domain of RVE domain. Special care should be taken on mesh refinement; mesh size should small enough to capture the location of material interface.

5.2 Gmsh for Geometrical Modeling and mesh generation on weave.

Gmsh, free finite element mesh generator software is used for constructing the geometry by using its geometry module. Gmsh is developed by Christophe Guzaine and Jean-Francois Remacle and the software is facilitated with four module named geometry, mesh module, solver module and post-processing module respectively. A computer program is written along with sub routines to generate a single fiber in weave in x-y plane as shown in figure 15 with various parameters that includes the width and thickness of fiber in x-y plane and out of plane respectively.

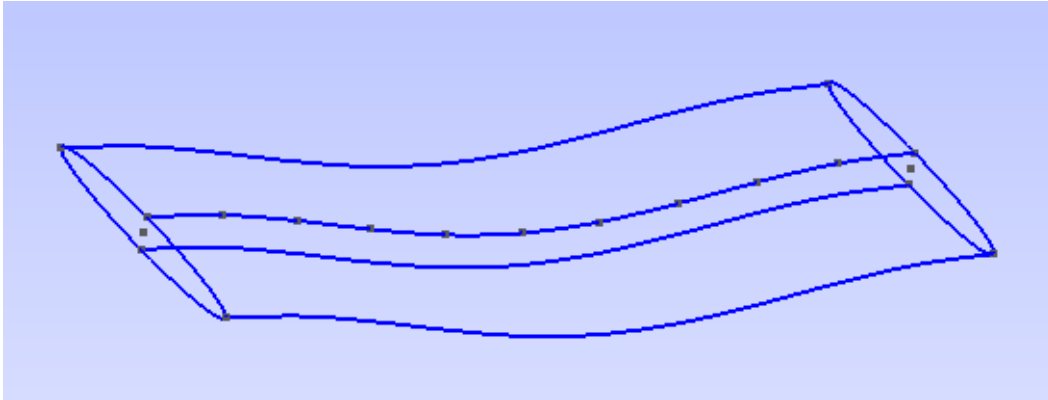


Figure 16: Single fiber geometry constructed in Gmsh

As it can be seen that cross sectional area of the fiber is elliptical that is constructed on both side by geometry module with the help of four points and then connected through the smooth curve by joining ten points along the length as shown in above figure.

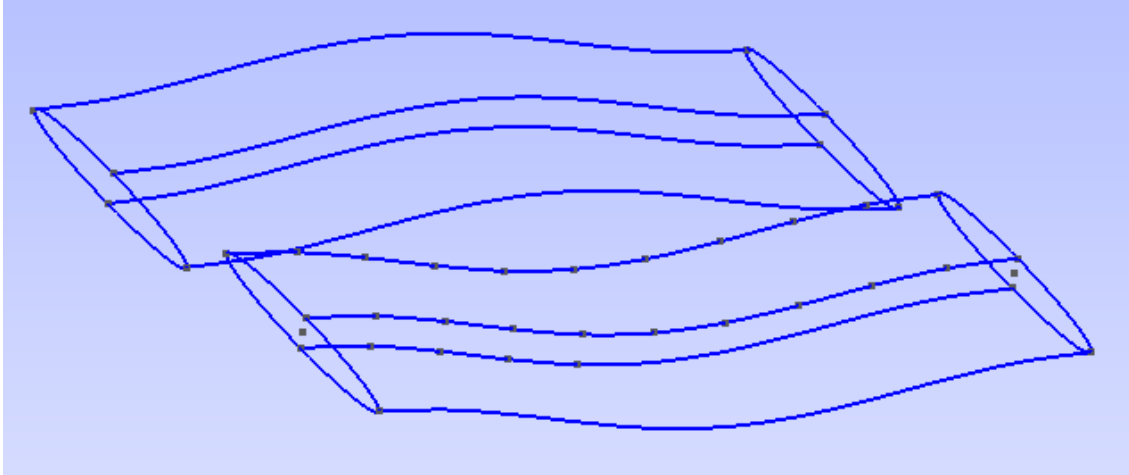
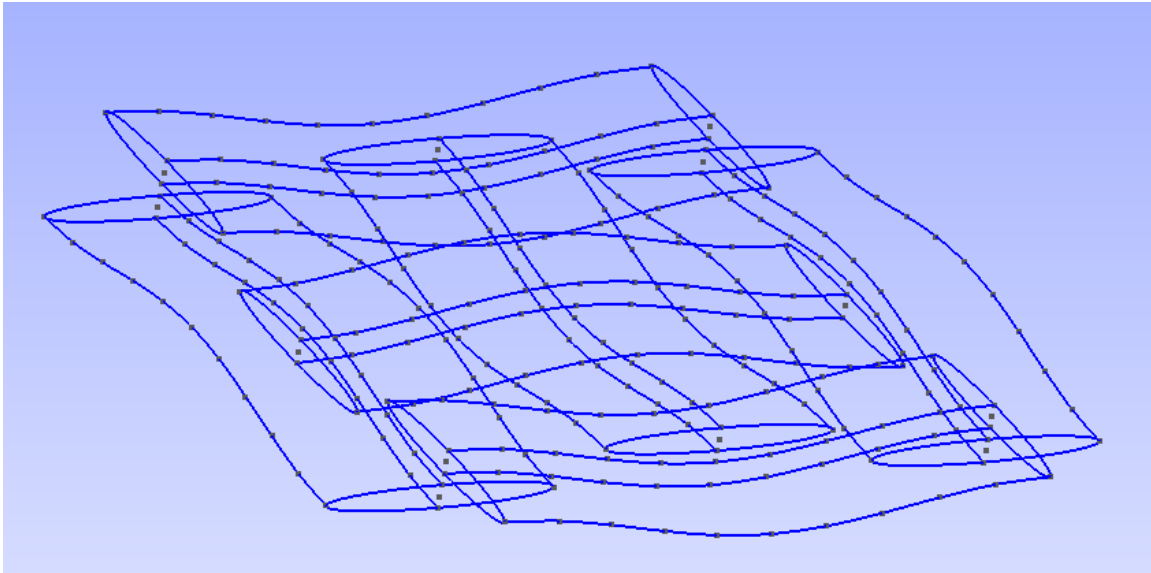


Figure 17: Spacing between two adjacent fibers in weave

Spacing between the fibers is also defined that can be seen in figure 16 that two adjacent fibers have certain spacing and there curvature is bending up and down respectively. All the inputs are user defined and can affect the size of fiber with change in values. Other set of variables are used for controlling mesh size e.g. number of mesh point along the length and elliptical cross section of fiber. Finally the complete geometry is shown in figure 17.



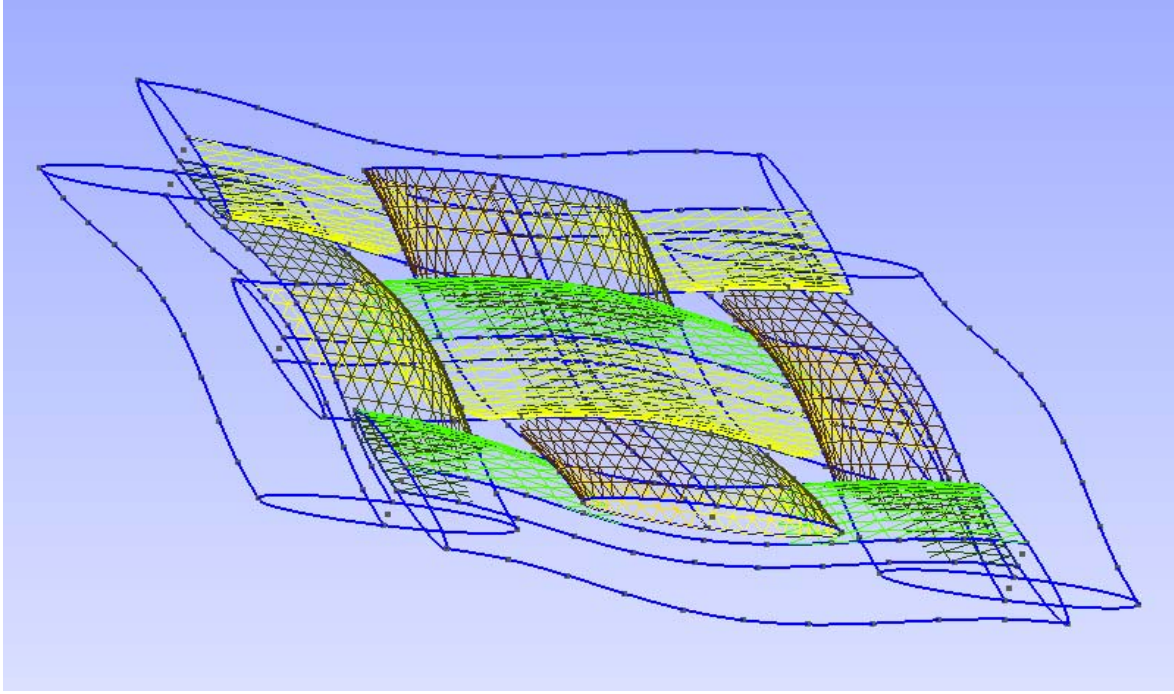


Figure 18 :(a) Complete geometry of fiber in woven weave (b) meshed surface

The mesh generating process is completed through Gmsh's mesh module with 2D triangular element options that generated a triangulated surface and a data sheet with description of number of nodes, their nodal coordinates, number of elements and element connectivity sequence.

5.3 Function and output of research code

A research code in MATLAB is written to generate a level set using RVE cell mesh from Gmsh. The MATLAB code reads the *.msh file* and collects all the nodal data description stated in the above section. A cubic voxel grid is constructed through a subroutine and discretized with equally spaced points and which is playing a role of matrix (binding) material of composite where woven shaped fiber is completely surrounded with these background points.

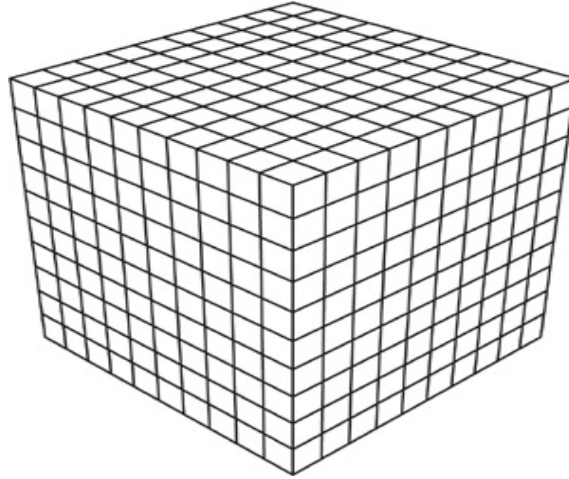


Figure 19: The uniform mesh used for level set and XFEM computation

The idea is to cover the whole length and width of fiber generated through CAD (Gmsh Software) with the surrounding equally spaced discretized points. It has already been mentioned that fiber is meshed with triangular elements. The surrounding points are used to calculate the discrete distance field. By distance field we understand a 3D grid of points where each voxel contains a scalar whose value is the shortest distance to the mesh.

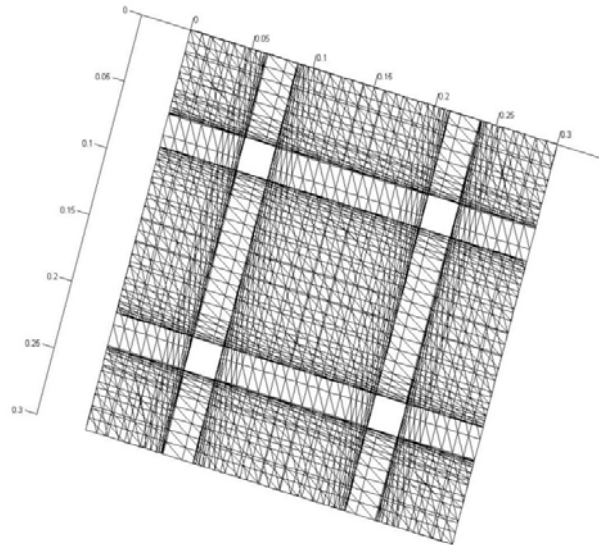


Figure 20: Meshed surface plotted in MATLAB

The sign (negative or positive) depends on the location of points whether it is below above or on the mesh. As we can see in figure below that mesh plot by MATLAB. In the figure 19 the top view of fiber can be seen having dimension 0.3×0.3 with 11552 elements and 6160 nodes.

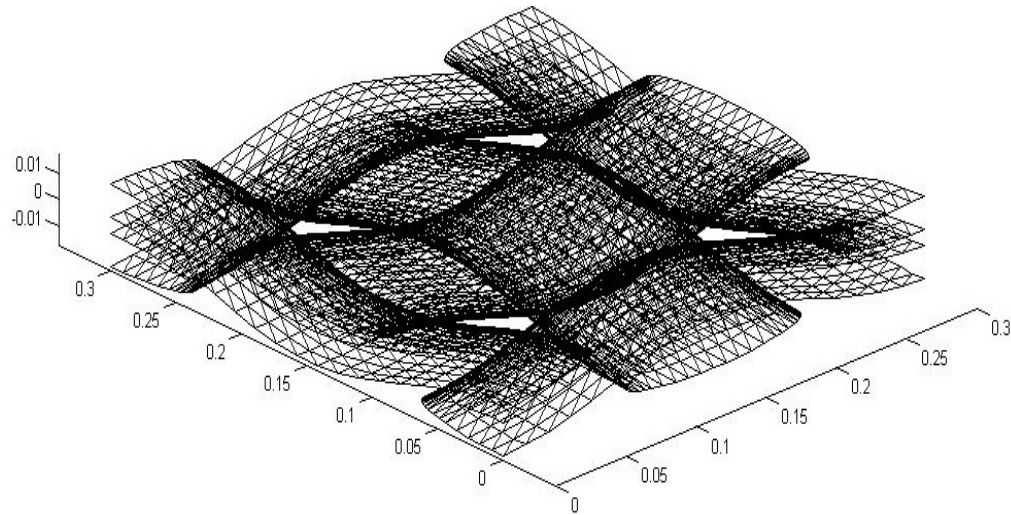


Figure 21: 3D view meshed surface in MATLAB

In the above figure the woven fiber surface in 3D, meshed with triangular element can be seen and compared with surface mesh done in NX shown in figure 20

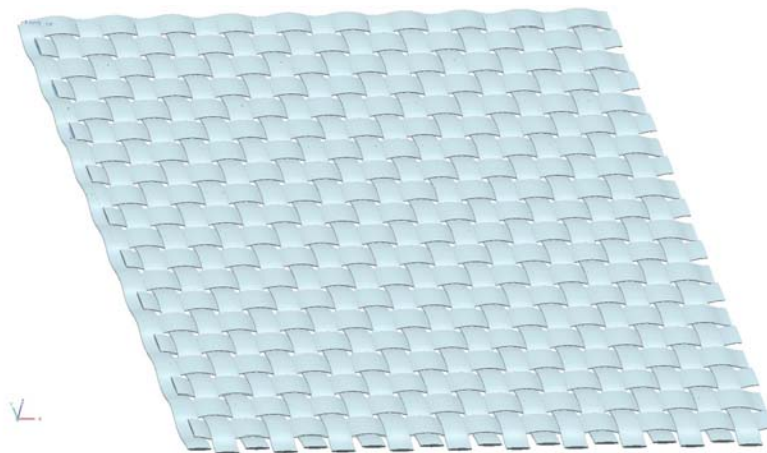


Figure 22: Fiber surface generated in NX

Now the intention is to completely confine this fiber (figure:) in cubical box of volume $0.3 \times 0.3 \times 0.3 \text{ unit}^3$ and discretized the whole cube with 8000 nodes that can act as voxel grid and MATLAB function is written for this purpose that can generate four node quad element structured mesh in 3D (cube or cuboids).

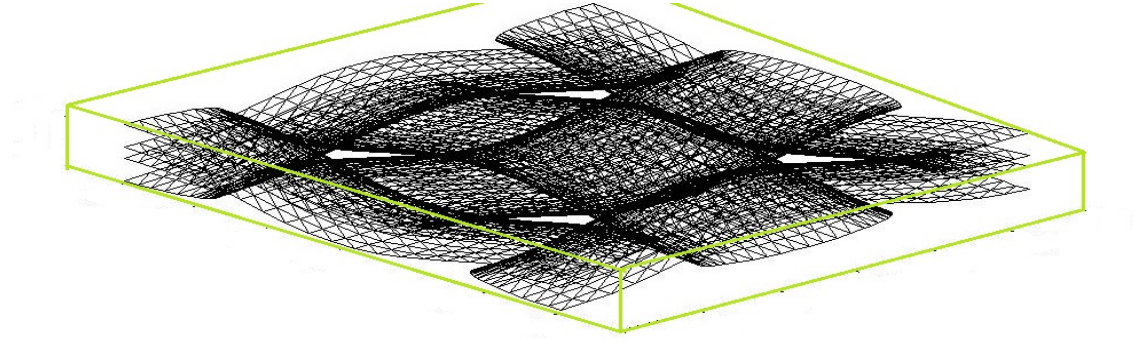


Figure 23: Confining the fiber into cube

With the help of these grid points a level set function from triangulated mesh is generated by computing the shortest distance from each grid point located above, inside or on the surface to the mesh. The calculation of signed distance and closest point from background points to the finite triangle is essential in order to gather the level set data and afterward the weave surface is tracked by plotting zero level set

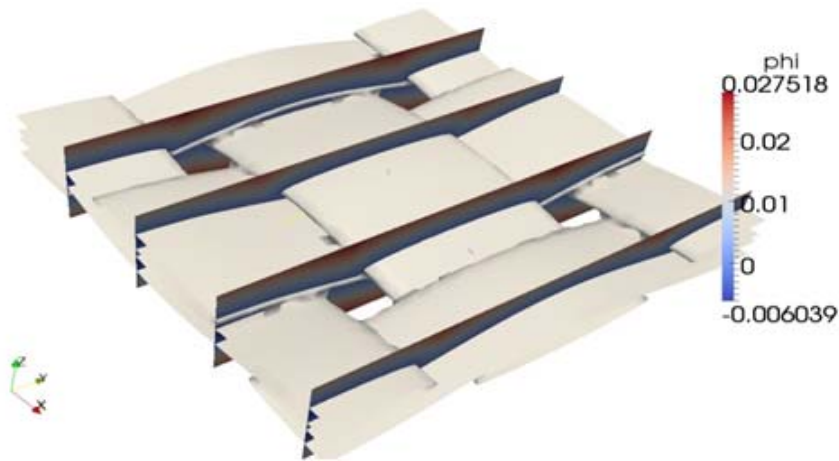


Figure 24: Level Set Plot for fiber as phi through C++ code

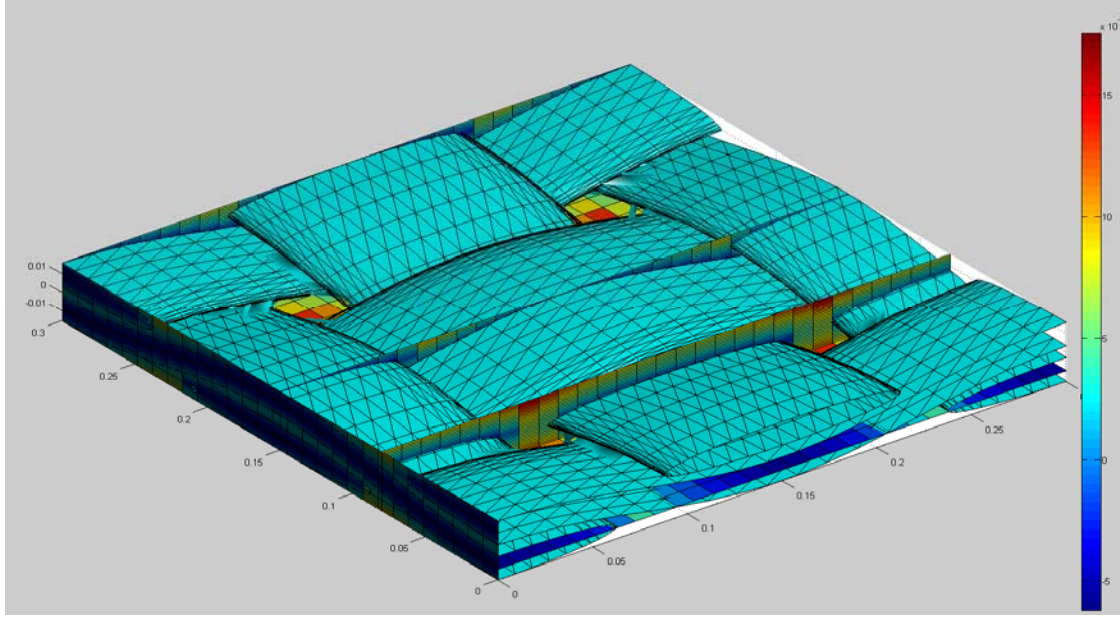


Figure 25: Level set plot through MATLAB

In figure 24 and figure 25 shows level set values is computed by using C++ code and MATLAB respectively. The level set values are defined over slice as counters with different numerical values indicating with different colors that can be referred with color bar placed at side of each generated fiber. As we can observe that level set with positive values are shown in red and negative values through shades of blues. e.g.: see the lower level of color bar. It can be seen that around the intersection of fiber and slice, zero level set is defined through color that holds the numerical value set to zero which represents the fiber surface.

Isosurface of the woven fiber is extracted from the volume data (Φ) to visualize the 3D volume bounded by the points of same constant magnitude. MATLAB provides several excellent volume visualization commands. MATLAB command “*Isosurface*” is used here to plot this figure that shows the zero isovalue

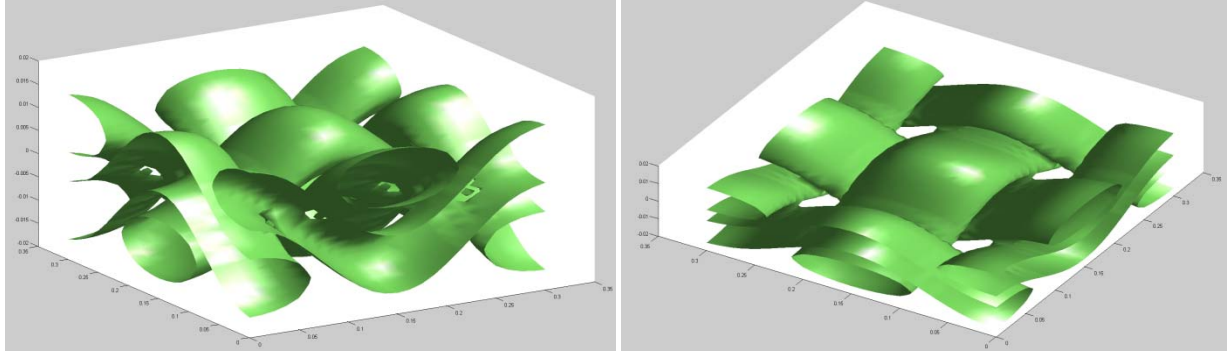


Figure 26: Isosurface plot with zero isovalue

The simulation is repeated with different number of grid points and it's been observed that computing time for level set increases significantly as number of grid points increases. It is advisable to have more grid points in order to plot zero level set but on the cost of high computing expenses. All the computation is carried out on SUN workstation at Computational Mechanics Lab-The University Of Texas at El Paso configured with 64-bit operating system, 4.00 GB installed memory (RAM) and two Dual core AMD Opteron 2222SE 3.00 GHz.

The following table shows time consumption with respect to number of grid point and fiber meshed with 11552 triangular elements.

Table 2: Number of grids vs Computing Time

Number of grid points	Time taken to compute Level Set	Number of triangular element
125	176.14	11552
1000	1306.89	11552
3375	4388.48	11552
8000	10430.89	11552
390625	20216.23	11552

Some more tests are performed to check the level set after changing the geometrical parameters like width of fiber and its thickness and following plots are found. A single fiber in weave is tested. In figure 27, meshed surface and its Isosurface having zero isovalue is shown.

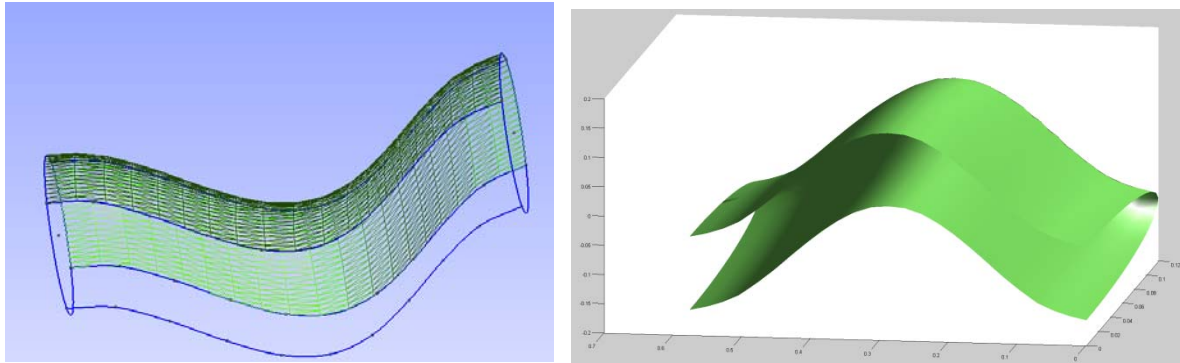
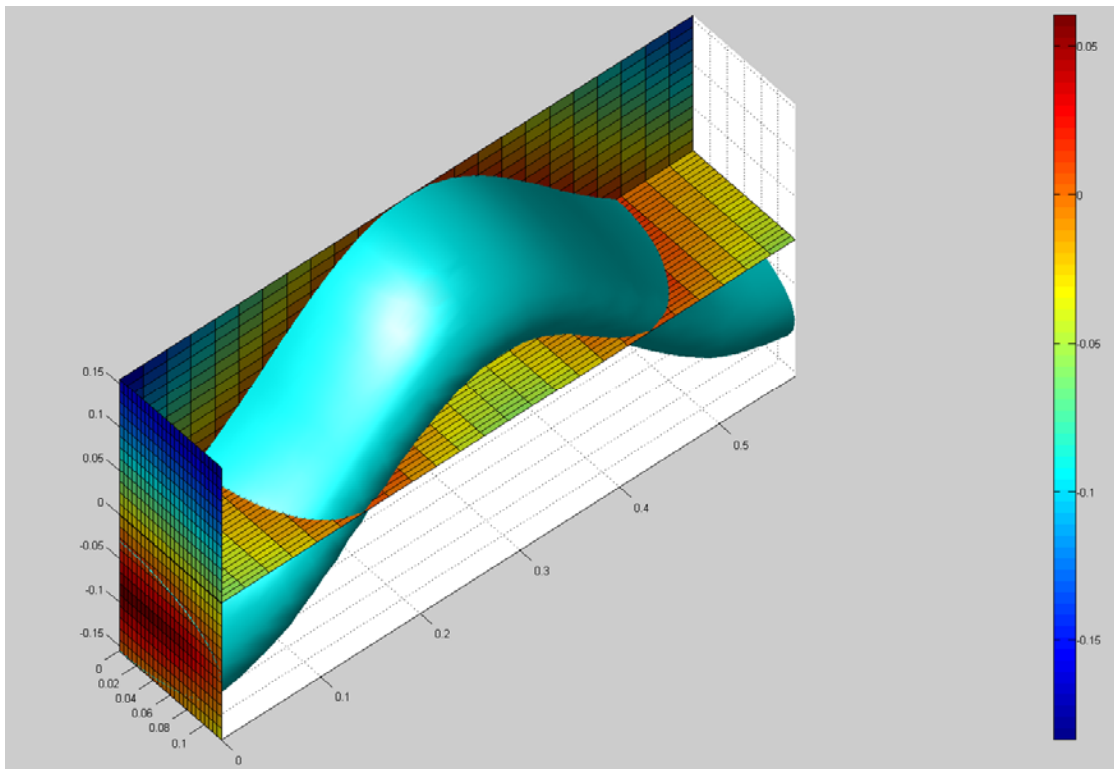


Figure 27(a) Meshed surface (b) Isosurface



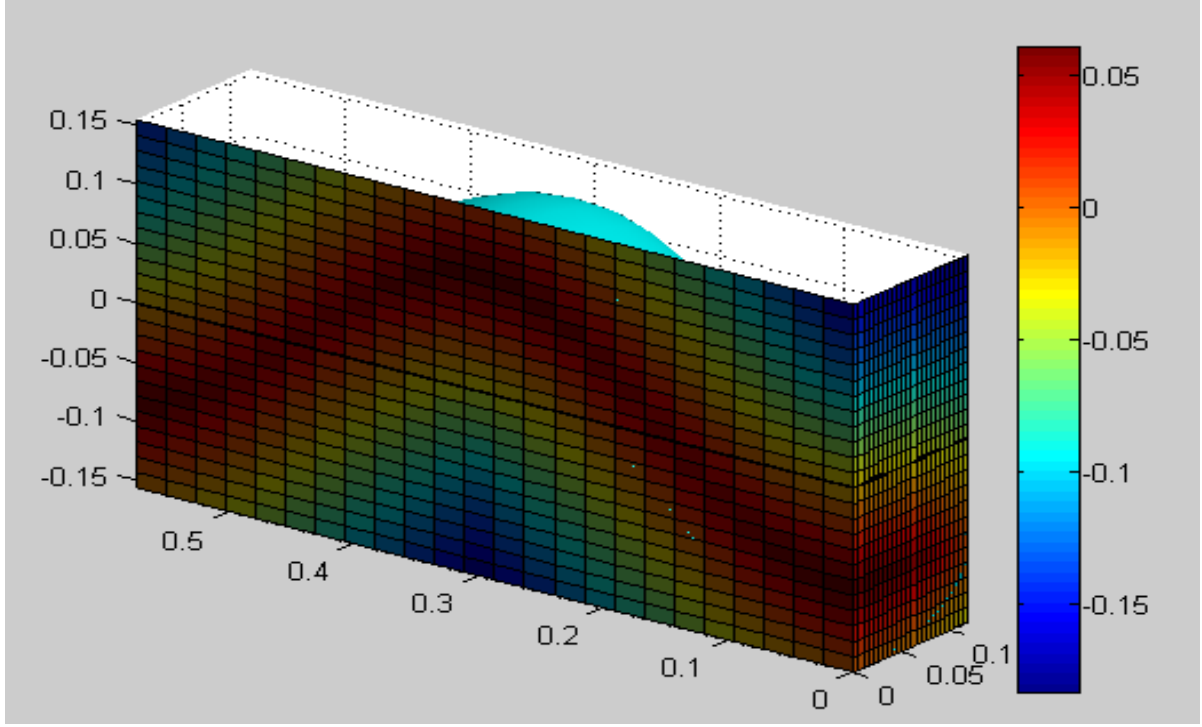


Figure 28: Zero level set plot of single fiber in weave

5.4 Background and computing concept of Distance fields

Letter M is used to denote a triangulated mesh which is a union of triangles T_i where $i \in [1, N]$ where N corresponds to the number of triangles. In other words

$$M = \bigcup_{i \in [1, N]} T_i$$

It is assumed that M is a closed in 3D Euclidean space. The important assumption [35] is stated that mesh doesn't contain any self intersection but triangle could share only edges and vertices. The other assumptions are enforced that edges must be positioned adjacent to exactly two triangles. The last condition is that triangles incident on vertex must form a single cycle around the vertex [35]. The conditioned and assumption mentioned above is important for determining the sign of distance field that informs the position of voxel whether it is outside or inside the closed, orientable manifold.

Now distance from every point in the grid to the mesh is required in order to generate a distance field that actually consists of shortest distance. The distance d from grid point P to the triangulated mesh M can be easily defined as

$$d(P, M) = \inf_{x \in M} \|P - x\|$$

The point on the mesh which is the closest to the point P , is considered as the closest point for this grid point P . As we know the mesh is the union of its triangle as represented in above equation where N is the number of triangle and T_i is triangle number. So

$$\begin{aligned} d(P, M) &= \inf_{x \in M} \|P - x\| \\ &= \inf_{x \in [1, N]} \left(\inf_{x \in T_i} \|P - x\| \right) \end{aligned}$$

In other words, from grid point the distance is computed to M by computing the distance from the point to every triangle in M and selecting the smallest distance to any triangle [35]

The next thing is to decide the position of closest point weather it is vertex, lies on edges or on the triangle itself and then the next question is how to compute the distance d . In the following section the sign computation and shortest distance computation subroutine is discussed.

5.5 Computing the sign distance and closest point from a point to finite triangle.

In this method, basically we check the position of points with respect to the outward normal to the triangle, since we have used triangular element in mesh and the sign convention is such that the sign is positive if the point is in the positive direction with respect to the outward normal and negative if point is in negative direction. The closest point could be the any of the three vertexes, on the edge which is a line segment or it could be anywhere over the triangle.

A subprogram is written in MATLAB in order to compute distance d from the point P to the finite line segment defined by its endpoints $n2$ and $n1$ as well as the point on the line segment that is closest to the point, let say cp .

Step 1: Calculate the Vector $u = n2 - n1$

Step 2: Calculate the vector $v = p - n1$

Step 3: Obtain the Cross product of vector u and v respectively

Step 4: Calculation of norm of vector u and v

Step 5: Check with conditional statement

```

IF [Cross product <= 0]
    d = norm (v) & cp = n1
ELSE
    Calculate [norm (u) ^2]
    IF [Cross product >= norm (u)^2 ]
        cp = n2
    ELSE
        cp = n1 + (Cross Product) * vector u / norm (u) ^2
        /* signifies that cp is on the line segment */
    END
    d = norm (p - cp)

```

5.6 Algorithm for computing level set function

The nodal coordinate data of each triangular element in mesh, element connectivity matrix and coordinates of voxel's point are collected as input arguments in order to generate a function for zero level set calculation. As we know zero level set represents the surface and positive if the point, on which level set is, calculated lies above the surface and negative if point lies below the surface.

Level set is computed on every point in grid so in order to make program executable the distance from each point to their triangle mesh is calculated and shortest distance is taken.

Function Phi= mshgenls (node, element, lspoints)

FOR i= 1 to [number of grid points, 1] /*matrix with one column*/

FOR e=1 to [number of elements, 1]

Collect nodal data of X -coordinate of all elements in variable n1

Collect nodal data of Y-coordinate of all elements in variable n2

Collect nodal data of Z -coordinate of all elements in variable n3

d = function for computing shortest distance to triangle (pt, n1, n2, n3)

/* where pt -> coordinates for grid point

n1, n2, n3 are vertex of triangle. */

IF [absolute value (d) < absolute value (dmin)]

dmin = d

END

END

Phi (i) = dmin

END

Chapter 6: Conclusion and Future Work

This work is an attempt to compute level set data for woven fiber having complicated geometry with the use of appropriate sign distance function that uses closest point method .Shortest distance from each grid point to every triangular element is computed to generate a distance field and associated signs shows the position of point weather it resides inside the fiber, outside the fiber or on the fiber. Eventually the fiber surface is represented by plotting zero level set. As we know the field quantities (stress, strain etc) never stay continuous at material interface so a discontinuity is expected in the form of jump and kinks in the strain field. XFEM is robust computational technique to handle these classes of problems where solutions contain discontinuities, discontinuities in gradient, singularities or boundary layer and interface problem can be solved through fixed grid method by enriching the elements that is cut by interface. The computed level set is required in order to construct the enrichment function of extended finite element approximation and to represent the surface independently.

Reference

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Vita

Himanshu Kumar was born in Patna, India on December 4th, 1983. He completed his Higher Secondary School Exam from Loyola High School, Patna, majored in math, physic and chemistry. He received Bachelor of Engineering degree in Mechanical Engineering from Bharati VidyaPeeth University, Pune in 2008. He moved to The United States of America in 2009 to pursue his Master of Science degree in Mechanical Engineering from The University of Texas at El Paso. During his master's, he worked as teaching assistant in the mechanical engineering department and as a research assistant in Computational Mechanics Lab and also a recipient of STEM scholarship in spring 2011. In summer 2011, he graduated from Master of Science degree in Mechanical Engineering from UTEP after successfully defending his thesis.