Failure of laminated composite materials - probabilistic analysis and machine learning [INT4]

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Introduction

Why Composite?

- Tailorable properties, with high stiffness, strength and lightweight characteristics makes it stand apart from its monolithic counterparts.
- Very high specific strength and specific modulus causes them to be as strong as metals with very low weight.
- Damping properties can be engineered as needed.
- Conductivity(Thermal and electrical) can be varied.
- High resistance to wear and corrosion

What are the problems associated with composites?

- Anisotropy (Direction dependent properties)
  - Requires highly complicated and difficult mathematics for analysis.
  - Much more costly and computation time required is not profitable.
- Non-homogeneity (Space dependent properties)
  - Due to their inherent nature of having different constituents combined macroscopically, there is difference in properties with respect to space.
- Stochastic variance in properties
  - Due to imperfections in fabrication, even orthotropic composites like laminates have differing properties along space, as well as batches of production
  - For example: The diameter of fiber is not constant everywhere, as well as the spacing between matrices is not constant.

Motivation for Project:

- Currently, the best and most reliable technique that exists for stochastic modeling of composites is Monte Carlo Simulation. But it requires a lot of data for giving reliable results.
- Come up with a state of the art approach to decrease the time and computational cost consumed by standard Monte Carlo Simulation method.
- Minimum number of experiments to be carried out to train the metamodel along with minimum error from values predicted from MCS.

Why Metamodels

Use of Metamodels is coming into picture nowadays as it:

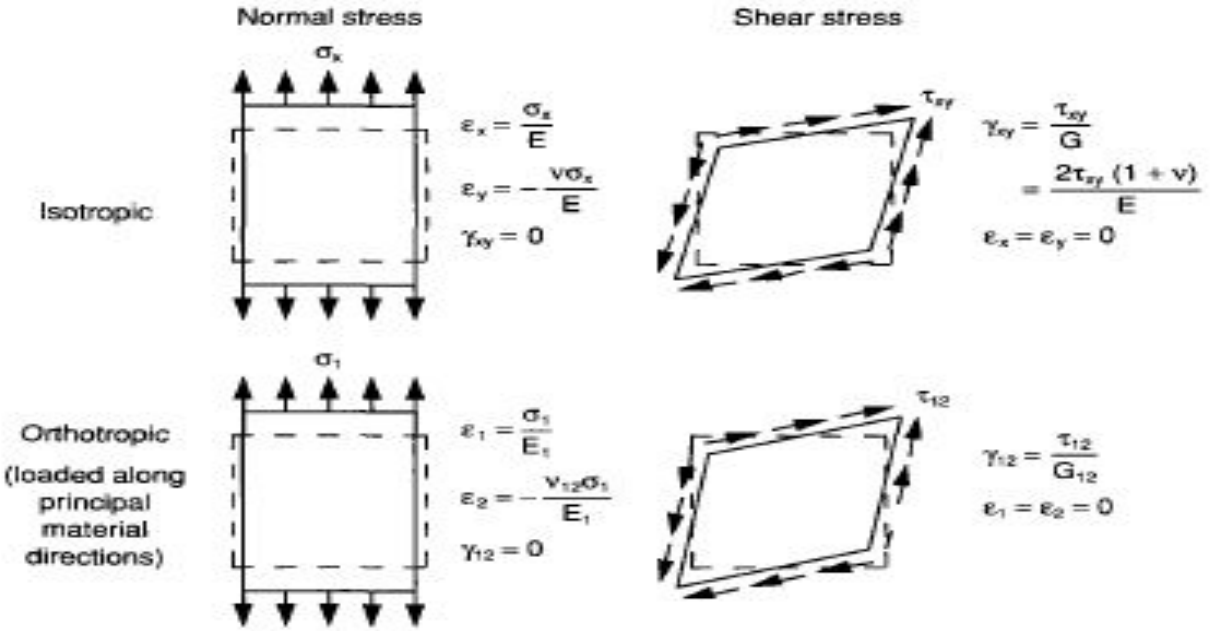
- Mimics the behavior of the model and gives accurate results.
- It is computationally inexpensive to evaluate.
- Access the uncertainties in Input variables and the same are quantified and fitted to a mathematical model.
- Requires less number of sampling points(selected through mathematical algorithm).
- Time efficient

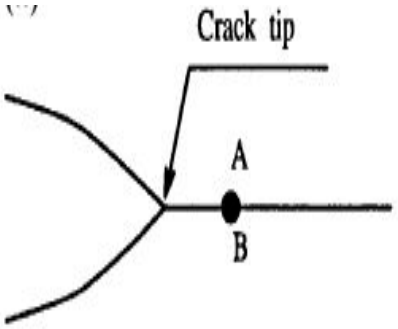
Literature Review

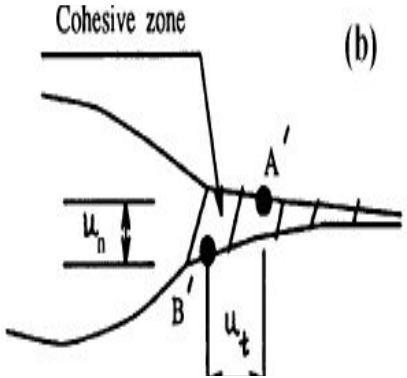
Variation of Properties in Composites

- In most traditional structural materials, their mechanical behavior is assumed to be homogeneous and isotropic but mechanical properties of composite materials exhibit intrinsic statistical dependence and generally assumed to follow Normal distribution.
- In particular, in-homogeneity, anisotropic characteristics and brittleness of the matrices and fibers affects strength of the composites at a significant level than any other property.

Literature Review



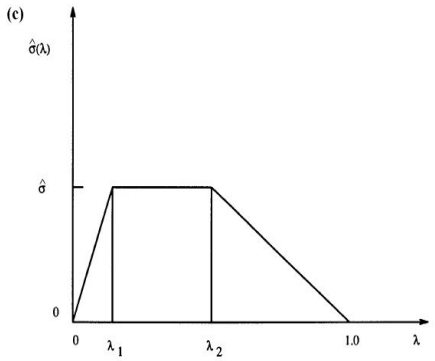




Cohesive Zone Model

- Major research in the area of fracture mechanics has been done on stationary cracks, which are not applicable to the crack propagation phase.
- In case of Composites, catastrophic failure of material is not due to initiation of crack but due to the stable crack propagation phase.
- Reserve strength in the system after the crack initiation is expended during propagation and finally fracture happens with catastrophic failure.
- Another important technique is the nodal release method, but it doesn't have a material length scale and hence strong dependence of FEA results on element size.

Cohesive Zone Model



- For analysis of reserve strength, its expenditure and the crack growth phase, cleavage plane is modelled as a Cohesive zone.
- Traction Separation law governs the mechanical response of cohesive interface. which relates traction force and separation parameter.
- With increasing interfacial separation, the traction across the interface reaches a maximum and then decreases to zero so that complete decohesion occurs.

Why bother about this variation

- Due to the uncertainties in the different parameters a component made of a composite may have a slight variation in properties like Young's modulus, Density, Modulus of rigidity etc.
- Similarly, when large number of composite components are manufactured, it is highly likely that their properties are slightly varying around the mean value.
- For such cases, it is hard to provide a deterministic answer whether a randomly chosen component will fail under certain loading conditions.

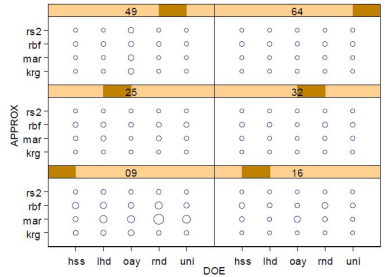
How to represent the uncertainty of the properties of composites

- Probabilistic methods are used to represent uncertain parameters.
- Probability distribution functions can be established for all uncertain parameters taking into account the correlations between different parameters.
- The result of the analysis can be interpreted in a statistical sense, and the probability of every output quantity depends on the input probabilities and their correlations.

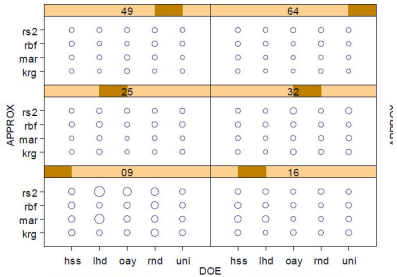
Monte carlo in Probabilistic Mechanics

One of the classical computational methods for measuring the uncertainty or probability of failure of any structure is Monte Carlo simulation where the repeated calling of random samples from the target population of input design parameters according to their distribution is used to plot a probability distribution graph and the further decision is made. A large number of calls that are required for precise predictions are usually not compatible with costly computational models such as finite element models, even when high-performance computing platforms are available at hand. However it is not preferred because:

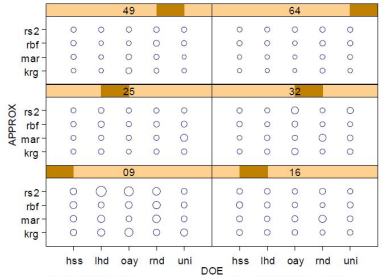
- High Computational cost
- Time consumption
- Random and Large quantity of Sample points
- Modeling all the correlations between variables



(a) RMSE for volume [FCN = 1]



(e) RMSE for stress constraint 2 [FCN = 3]



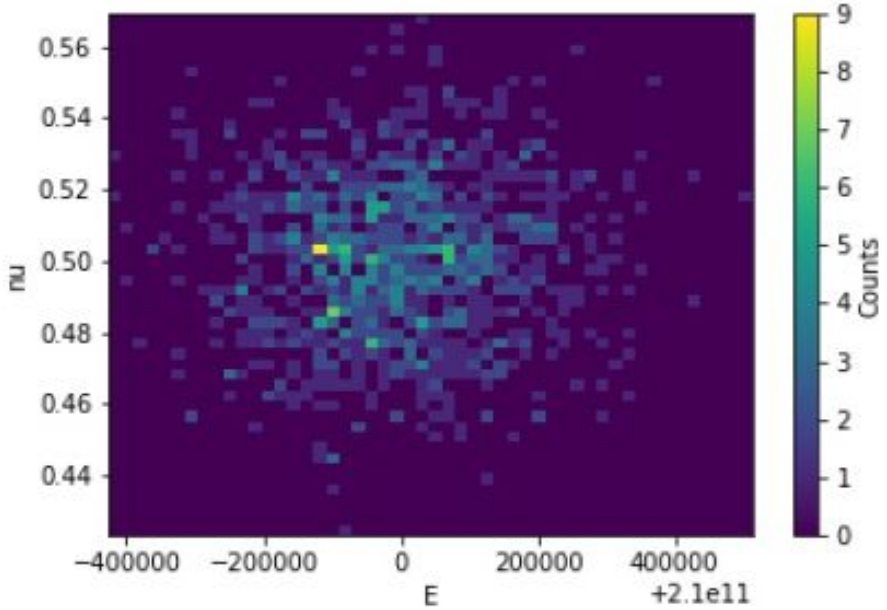
(c) RMSE for stress constraint 1 [FCN = 2]

Metamodels survey

As from the literature, it was observed that

- The **kriging models** tends to offer more accurate approximations over a wide range of DOE types and SAMP sizes.
- Also **Hammersley sampling sequences** tend to yield more accurate approximations globally as indicated by the consistently low RMSE values. Although MAX values are somewhat compromised.
- SAMP size generally show upward trend for more accuracy. However for low-order non-linear functions, large sample does not improve accuracy that much.

Random sampling technique



Frequency contour plot for E and nu for 2D normal distribution

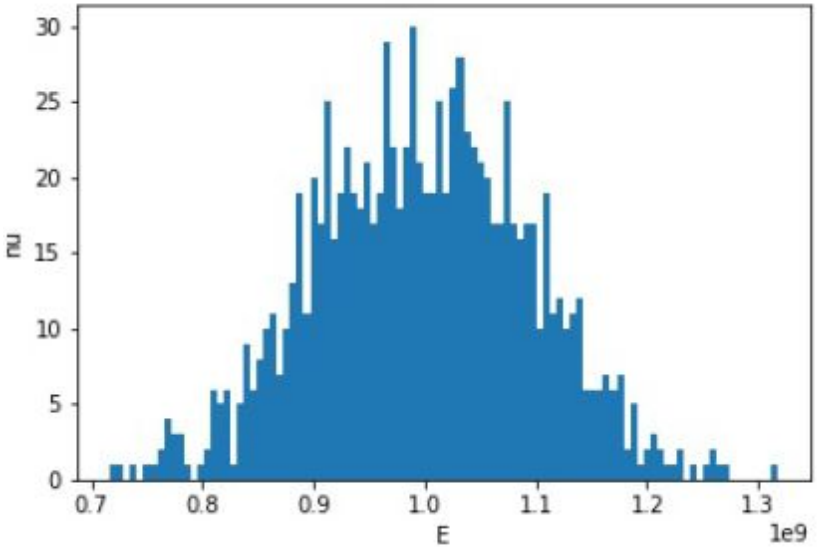
- Recall the pdf for the MVN distribution

$$\phi(\mathbf{x}) = \frac{1}{2\pi^{\frac{p}{2}}|\Sigma|^{\frac{1}{2}}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})' \Sigma^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}$$

- Where
  - $\mathbf{x}$ is a p-length vector of observed variables
  - $\boldsymbol{\mu}$ is also a p-length vector and $\mathrm{E}(\mathbf{x})=\boldsymbol{\mu}$
  - Σ is a pxp matrix, and $\mathrm{Var}(\mathbf{x})=\Sigma$
    - Note, Σ must also be positive definite

MVN(Multivariate Normal) Distribution:
x= {E, nu} and **Σ** = 2*2 covariance matrix

Random sampling Technique

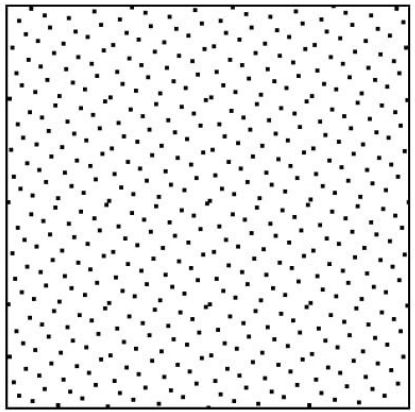


Frequency contour plot for E for 1D normal distribution

For 1D it is very simple, we just have to know the variance and mean value of Young's modulus.

But for 2D, we have to get the covariance matrix, in which not only the variation in respective properties is needed, but also the dependence of one property on another. Usually one derives this matrix on the basis of experimental data, but we didn't have the time to conduct experiment. So we assumed the covariance matrix.

Hammersley Sampling Technique



Algorithm used is:

Each non-negative integer k can be expanded using a prime base p:

$$k = a_0 + a_1 p + \ldots + a_r p^r$$

where each a_i is an integer in [0,p-1]. Now define a function Φ_p of k by

$$\Phi_p(k) = a_0/p + a_1/p^2 + \ldots + a_r/p^{r+1}$$

k-th d-dimensional Hammersley point is

$$(k/n, \Phi_{p1}(k), \ldots\ldots, \Phi_{pd-1}(k)) \quad \text{for } k = 0, 1, 2,..., n-1$$

Finite element analysis

Finite element analysis is an effective, method of numerically solving many types of differential equations.
We decided to use this technique to generate the training, cross validation and test data required for metamodel training. FEA is best choice for us because:

- We will not be able to get results for exact properties as found from sampling techniques.
- The timeframe of research is not enough for conducting large scale experiments.
- Also, a custom model will help us tweak the parameters much easily. We will also explore some existing libraries and Abaqus python extension for the same.

Object oriented modeling of Finite elements

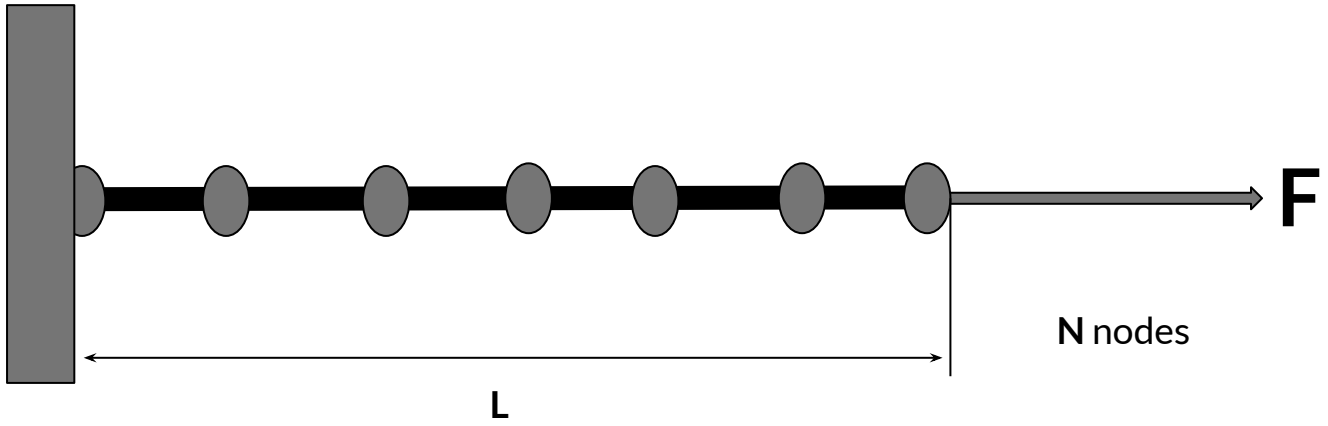
The steps involved in Finite Element Modeling are as follows:

- Discretization
- Assembling
- Solution

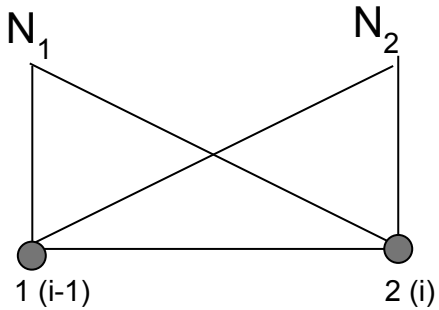
A typical discretization programme contains:

- Scalar parameters (number of nodes, number of elements etc.)
- Material properties
- Coordinates of nodal points
- Connectivity array for finite elements
- Arrays of element types and element materials
- Arrays for description of displacement boundary conditions
- Arrays for description of surface and concentrated loads

1D FEM



Boundary conditions: $\begin{cases} x=0,\ u=0 \\ x=L,\ \text{Force} = F \end{cases}$



i^{th} element

We used linear shape functions to approximate the residue and weight functions: $N_1 = x_{local}$ and $N_2 = 1\text{-}x_{local}$.

$U = S - WD_{EF}$, ($WD_{EF} = 0$ is assumed)

S is local stiffness matrix.

$$S = 0.5\int^{L}_{0}\varepsilon^{T}_{x}\sigma_{x}A\,dx$$

$$\Rightarrow S = 0.5\int^{L}_{0}\varepsilon^{T}_{x}E\varepsilon_{x}A\,dx$$

$$\Rightarrow S = 0.5AE\int^{L}_{0}[u]^{T}[B]^{T}[B][u]\,dx$$

To minimize U, dU/d[u] = 0, here we get local stiffness matrix: $[k]_{local} = (AE/L)[[1\ -1],[-1,\ 1]]$.

After this, we calculated the Global stiffness matrix in the assembling process. $[k]_{global}$.

Now, we applied the boundary conditions to the equation [k][u] = [F] and solved for [u] to get the displacements at various nodes.

Theoretical formulation of 2D plane stress problem

Equations of Motion

$$\frac{\partial \sigma_x}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} + f_x = \rho \frac{\partial^2 u}{\partial t^2}$$

$$\frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_y}{\partial y} + f_y = \rho \frac{\partial^2 v}{\partial t^2}$$

Stress Strain Relations

$$\begin{pmatrix} \sigma_x \\ \sigma_y \\ \sigma_{xy} \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & 0 \\ C_{21} & C_{22} & 0 \\ 0 & 0 & C_{66} \end{pmatrix} * \begin{pmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ 2\epsilon_{xy} \end{pmatrix}$$

Strain Displacement Relations

$$\epsilon_x = \frac{\partial u}{\partial x}, \epsilon_y = \frac{\partial v}{\partial y}, 2\epsilon_{xy} = \gamma_{xy} = \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}$$

2D FEM

Preprocessing

- Due to lack of time, we couldn’t patch our preprocessing code with our FEA code. We used ABAQUS input files to obtain the connectivity matrix and nodal file.

2D FEM

We used the following equations to compute element level stiffness matrices.

$$\implies \int_{\Omega^e} -W_1 \frac{\partial F_{12}}{\partial y} d\Omega = \int_{\Omega^e} \frac{\partial W_1}{\partial y} F_{12} d\Omega - \oint_{\gamma^e} W_1 F_{12} n_y ds$$

where, $F_{11} = C_{11} u_x + C_{12} v_y$, $F_{21} = C_{66}(u_y + v_x)$

$$\int_{\Omega^e} -W_2 \frac{\partial F_{21}}{\partial y} d\Omega = \int_{\Omega^e} \frac{\partial W_2}{\partial y} F_{21} d\Omega - \oint_{\gamma^e} W_2 F_{22} n_y ds$$

where, $F_{21} = C_{66}(u_y + v_x)$, $F_{22} = C_{12} u_x + C_{22} v_y$

We then converted these equations to normal form and used Gaussian Quadrature with two points per element for numerical integration.

2D FEM

We used the below algorithm to calculate global stiffness matrix from local stiffness matrix.

Algorithm 1 The direct stiffness method of finite element assembly

Ensure: $A = [0], F = [0]$
  for all $elementse \in \varepsilon$ **do**
    $(A^e, F^e) \leftarrow elem(e)$
    for all $localdegreesoffreedomd_1ofe$ **do**
      $F(L(e, d_1)) += F^e(d_1)$
      for all $localdegreesoffreedomd_2toe$ **do**
        $A(L(e, d_1), L(e, d_2)) += A^e(d_1, d_2$
      end for
    end for
  end for

Here, L(i, j) is Location matrix. For equations involving a single variable, L = Connectivity matrix. When More than one variable is involved, we have to generate the location matrix using the following algorithm:

2D FEM

Algorithm 2 Generate Location matrix

Require: $n_e \leftarrow No\_elements$
Require: $n_{pv} \leftarrow No\_Primary\_vars$
Require: $n_n \leftarrow Nodes/element$
Require: $M_C \leftarrow ConnectivityMatrix$
Ensure: $L = [O]_{n_e \times n_n \times n_{pv}}$, $A = [\,]$

```
j ← 1
for all i in n_e do
    A ← A + [j : j + n_pv]
    j ← j + n_pv
end for
for all i in n_e do
    k ← 0
    for all l in n_n do
        L(i, k : k + n_pv) = A(M_C(i)(l), M_C(j)(l))
        k ← k + 2
    end for
end for
```

Computations and Calculations

We performed Monte Carlo Simulation of finite element analysis on the following problem 1000 times. We determined the maximum displacement magnitude for each iteration. Using actual experiments, we can determine the threshold displacements above which the material can fail.

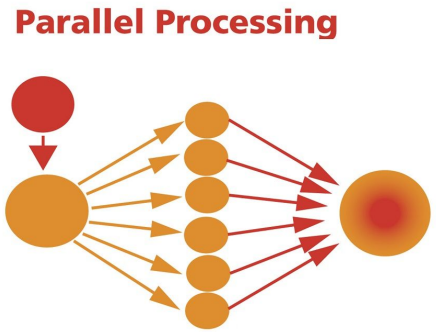
After that we extracted 50 and 100 data points using Hammersley technique for the same quantity to train the Kriging model.

3D FEM

- Extended the finite element model from 2D to 3D.
  - Derivation of continuous solution by using Equations of motion, Stress-strain relationships and strain displacement equations in 3D.
  - Discretization of the solution using shape functions in 3 variables.
  - Gauss-Legendre numerical integration for getting element level stiffness matrix.
  - 3D assembly algorithm to assemble the local stiffness matrices into global stiffness matrix.
  - Application of boundary conditions.
  - Find the displacement in 3D by solving for K and F.

- Crack initiation modeling
  - Duplicate elements on the site of the crack
  - Add new node index to set of nodes on either side of the crack
  - Change the corresponding element details in the connectivity matrix
- Crack propagation modeling
  - Initiate crack
  - Run FEM calculations
    - If resultant fracture strength of the common element is more than the prescribed limit, It means the material has debonded at that location.
    - Propagate crack
  - Iterate till all the values are in prescribed limits
  - Heavily resource intensive, multiple iterations of FEM required for obtaining the stimulation. Hence, Parallelization is required.

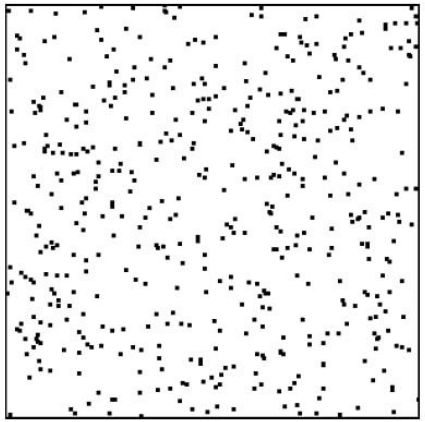
Parallelization



- More the number of elements in FEM model, better is the accuracy of results.
- Major downside of large number of elements in FEM model is that the time required for each simulation increases with increase in number of elements.
- Advantages of modelling FEM in Python includes customizations to the model as per need and faster simulations than the softwares available such as Abaqus.
- In crack propagation, multiple iterations are needed, which is highly compute power intensive.

- Stiffness matrix of each element requires numerous matrix operations which consumes most of the simulation running time.
- Several operations and functions can be run simultaneously on all or some of the cores of the CPU, which effectively reduces the amount of time taken for each simulation.
- For instance if a simulation is run on a system with octa-core processor and every core is involved in parallelization of code, then simulation time will be effectively reduced by 8 times.

Sampling Points:



For sample space to be covered uniformly by our data points, they should be uniformly distributed over surface. Random points might lose some significant property distribution over space.

Hammersley sequence is a low-discrepancy method which covers the sample space uniformly.

Kriging

kriging model postulate is a combination of a polynomial model and departures of the form:

$$\hat{y} = \sum_{j=1}^{k} \beta_j f_j(x) + Z(x),$$

Z(x) is assumed to be a realization of a stochastic process with mean zero and spatial correlation function given by:

$$\mathrm{Cov}[Z(\mathbf{x}_i), Z(\mathbf{x}_j)] = \sigma^2 \mathbf{R}(\mathbf{x}_i, \mathbf{x}_j),$$

where σ2 is the process variance and R is the correlation(gaussian generally)

Numerical Formulation

Post midsem

- Random sampling of properties from normal distribution
- Hammersley sampling for 2D
- 2D FEA model for isotropic materials
- Monte Carlo Simulation for 2D
- Metamodeling using Kriging for 2D and 1D

Numerical Formulation

Pre midsem

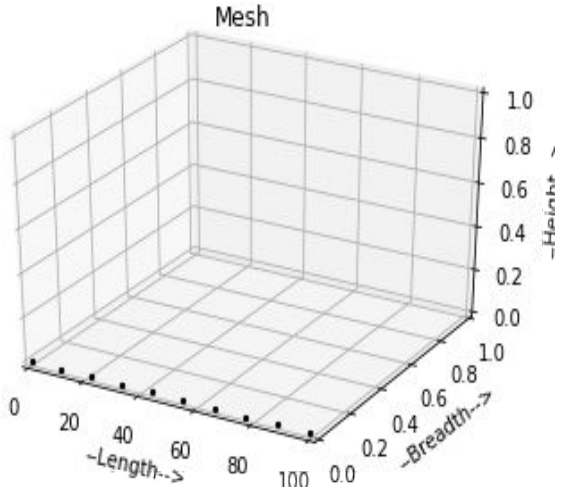
- Pre processing programme
- Hammersley Sampling for 1D
- 1D FEA model for isotropic materials
- Monte Carlo Simulation for 1D

Step by step procedure

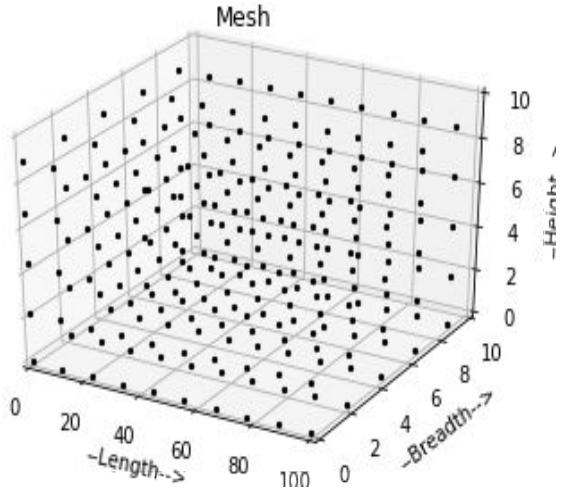
Three major tasks of the experiment was to:

- Get algorithmically selected input points which will be the training data-set for our model, through some sampling technique.
- Generate output for corresponding sampled points using FEA.
- Select an appropriate Metamodel to predict the output probability with least error as compared to standard results from MCS.

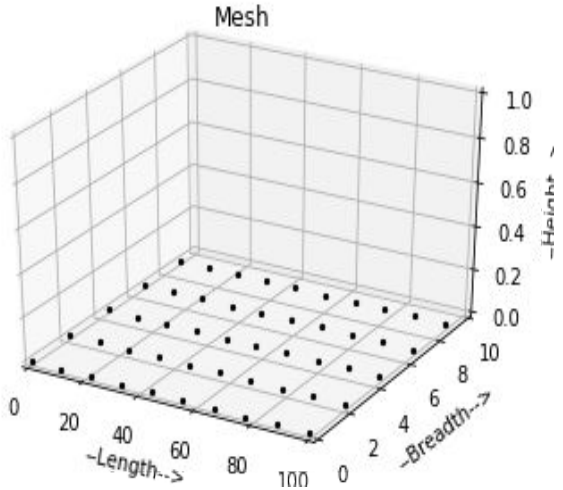
Results of Node generation programme



1D Mesh, 100 units long, 10 elements

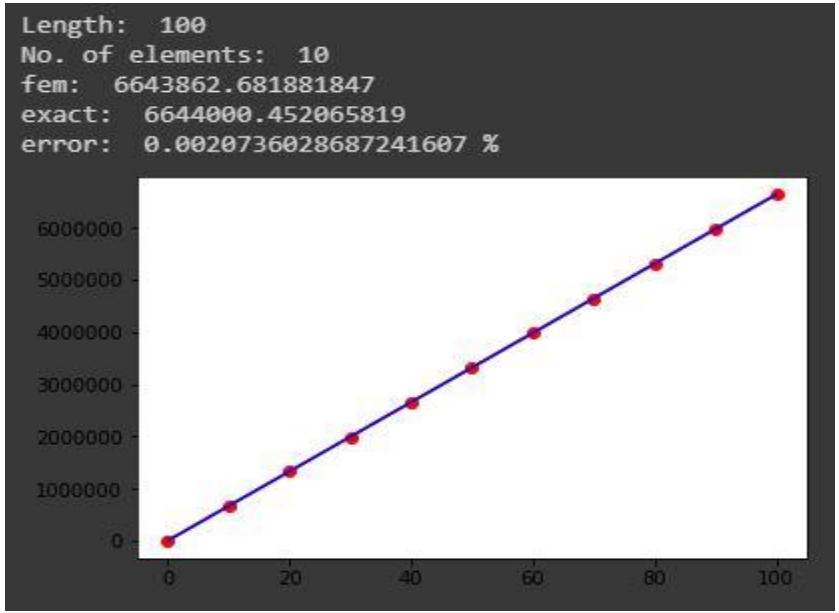


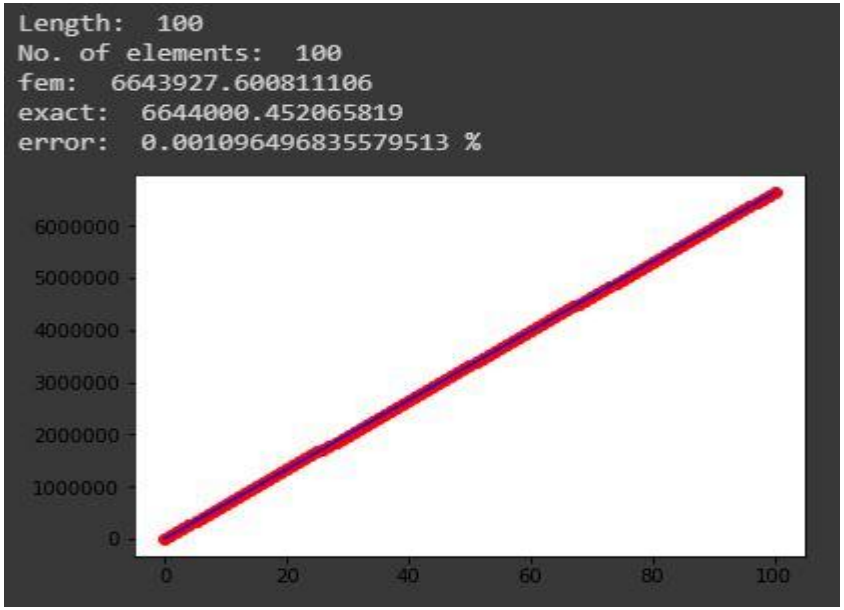
3D Mesh, 100x10x10 units, 10x5x5 elements



2D Mesh, 100x10 units, 10x5 elements

Results of FEA on 1D Bar





This figure denotes that accuracy of the FEA model increases as the number of elements increased.

2D FEM

We used the above example to conduct our FEA. The dimensions are l:b:h::1m:0.25m:5e-9m (Plane stress problem) , Mean E = 210e9, mean nu = 0.5. Variance in E and nu=10%, correlation in E vs nu and nu vs E to be 0.0001 and 1000 respectively.

Results

- We modeled the same mean parameters in ABAQUS and calculated the displacement to corroborate with our experimental FEA results. Our models come out to be accurate.
- We also did the calculation analytically by hand and the results are the same.

Results

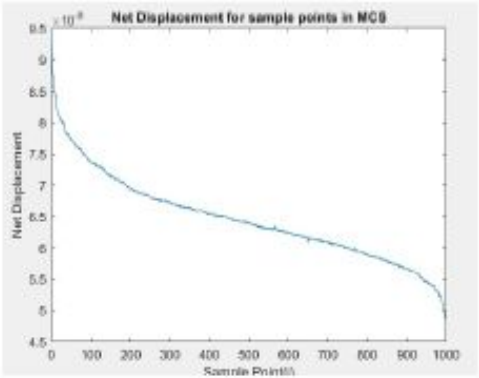


Fig. 3.9 MCS Plot

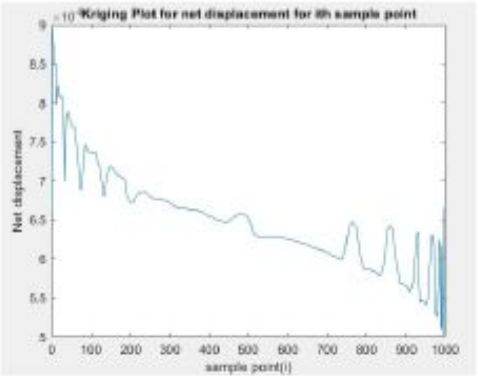
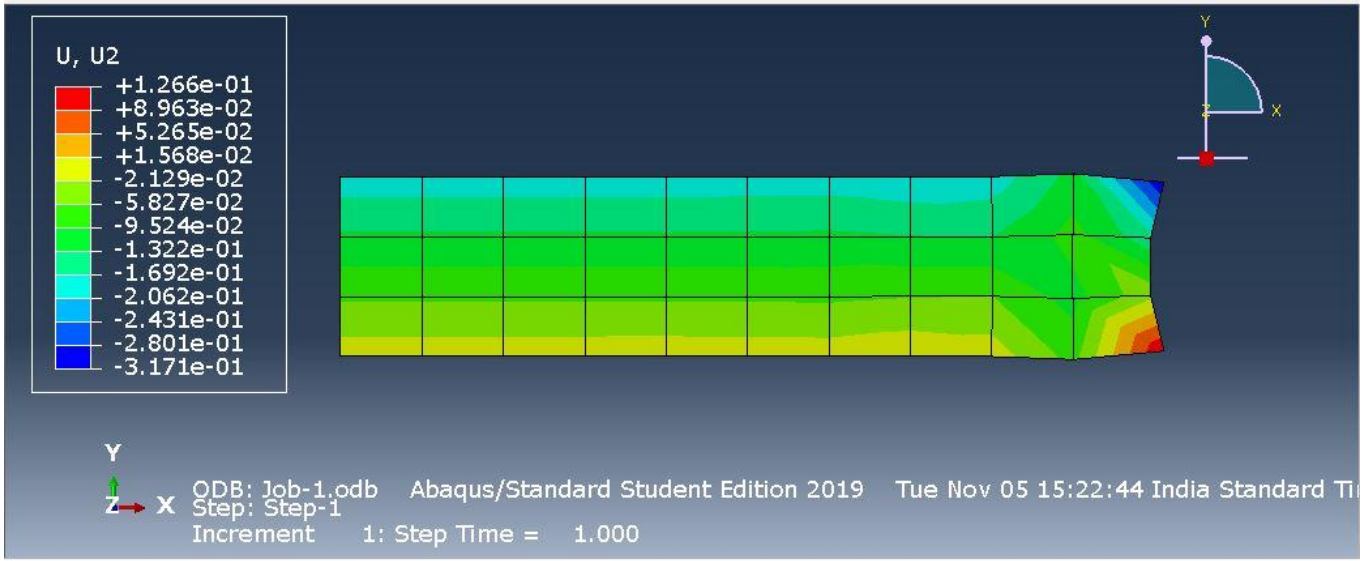


Fig. 3.10 Kriging Plot

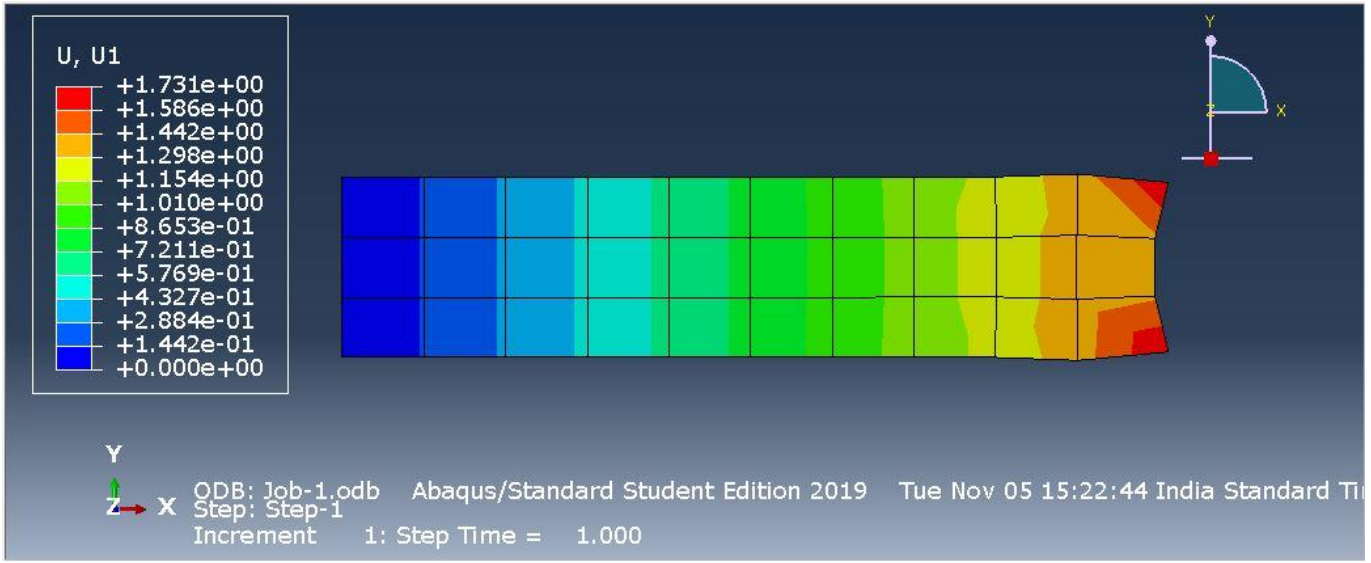
Comparison of results which we got from Kriging model with the results obtained from Monte Carlo Stimulation.

For 1000 sample points MCS predicted 45% probability of failure while our Kriging Metamodel predicted 51% failure.

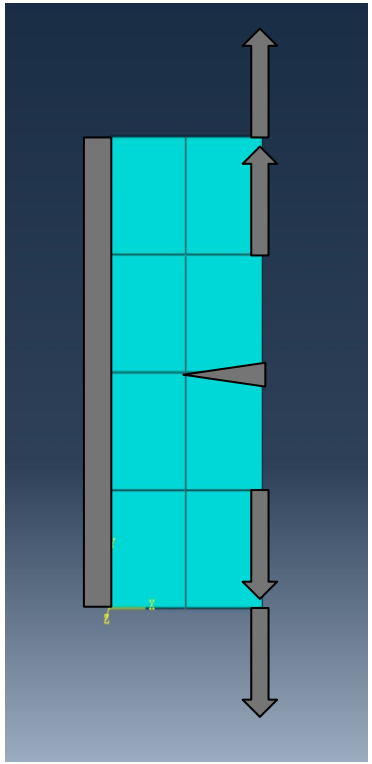
Contour plots of u_y

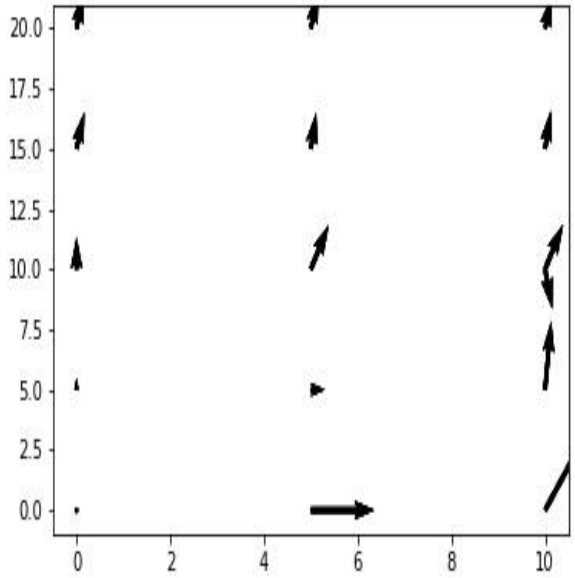


Contour plots of u_x



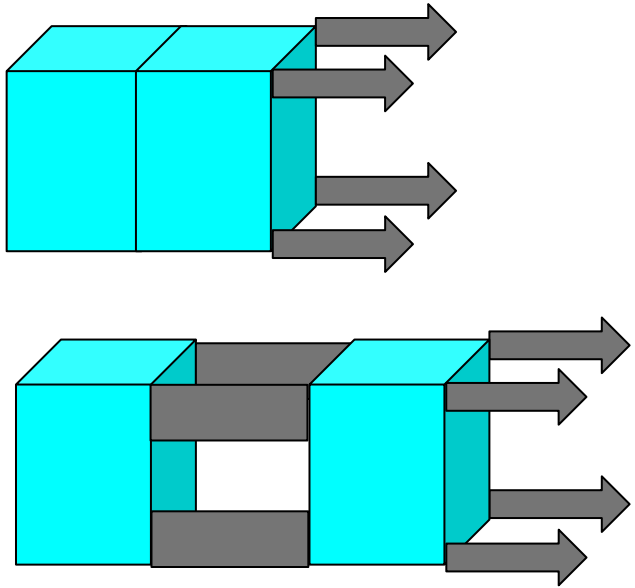
Crack initiation exercise





The vectors are showing displacement of nodes from initial to final position

Cohesive zone modeling exercise



Approximating the linear part of CZM model with springs attached to the two elements with const. k

Conclusion

- The research work carried out in this project provided us with an overview of metamodeling techniques and sampling techniques as an alternative to Standard Computational programs.
- The Kriging metamodel did give us acceptable likelihood of failure(51% vs 45% for MCS) but the L2 norm was not as expected.

Conclusion

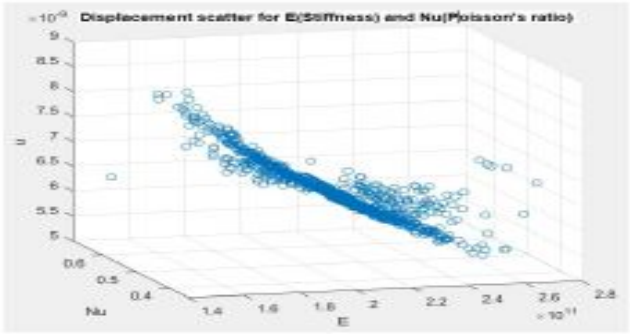


Fig. 3.7 Scatter plot for 2D displacement calculated by MCS

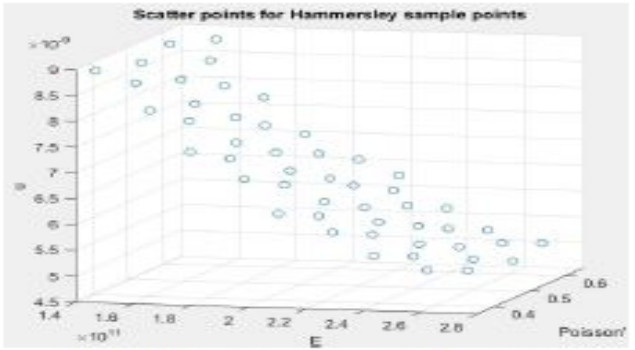


Fig. 3.8 Scatter for displacement from Hammersley Sequence points

In this plot we can clearly observe that there exists a pattern between the properties and the failure condition. Modern machine learning models like have the capability of detecting these patterns and we are hopeful that as the number of variables involved increase(which we will pass as features to the models), we will see improved prediction performance.

Future work

- Implementation of CZM and Crack Propagation in the 3D FEM code.
  - Integrate libraries for coarse mesh generation with our code.
  - Implement **parallel processing** to utilize the available compute power in multiple cores simultaneously.
  - Create methods for automatic crack initiation and propagation and modeling property variation wrt space.
  - Solve nonlinear problems associated with CZM.
- Literature survey to decide sampling techniques.
  - There are multiple independent and correlated material properties which we need to model. Planning to see if the currently used algorithms will scale up or not.
- Data generation -> Training Machine learning and Deep learning models on the data.
- Comparison and benchmarking.