B.Tech. Project
Data Driven Modelling of Composites

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End Term Evaluation

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Introduction

Composites -

A composite is a material made from two or more constituent materials with significantly different physical or chemical properties that, when combined, produce a material with characteristics different from the individual components. The individual components remain separate and distinct within the finished structure. The new material may be preferred for many reasons, primarily to maximize the useful properties and minimize the weaknesses of constituent materials; common examples include materials which are stronger, lighter, or less expensive when compared to traditional materials.

Applications

Airbus A380

More than 20 % of the A380 is made of composite materials, mainly plastic reinforced with carbon fibres. The design is the first large-scale use of glass-fibre-reinforced aluminium, a new composite that is 25 % stronger than conventional airframe aluminium but 20 % lighter.

Applications

Automobiles

Composites are being used increasingly in the automotive industry due to their strength, quality and light-weight. The materials used in automotive engineering play key roles in making lighter vehicles and ultimately lower emissions.

Applications

Wind Turbine

Currently, carbon fiber is used primarily in the spar, or structural element, of wind blades longer than 45m/148 ft, both for land-based and offshore systems. The higher stiffness and lower density of CF allows a thinner blade profile while producing stiffer, lighter blades.

Challenges

Since precise material properties are often needed to satisfy industrial needs and criteria, design of composites with **tailored properties** is of utmost importance.

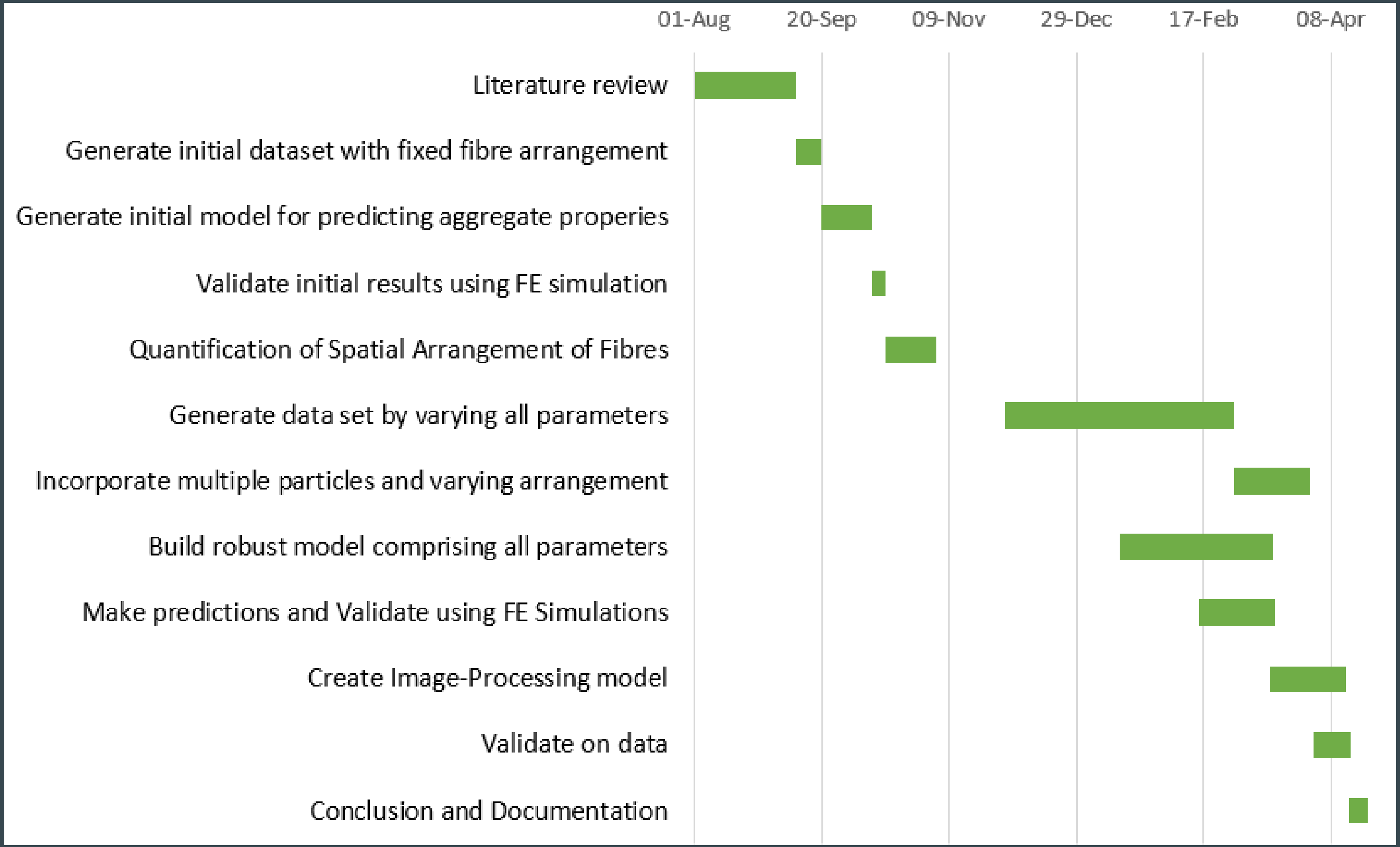
The design and analysis of such composites faces following challenges -

- Computational Expense
- Heavy Simulations
- Rigorous Experimentation
- Time Expensive Process

Project Objective

To develop an algorithmic framework to predict properties of composites to aid in meta-modelling process.

Project Timeline



General Workflow

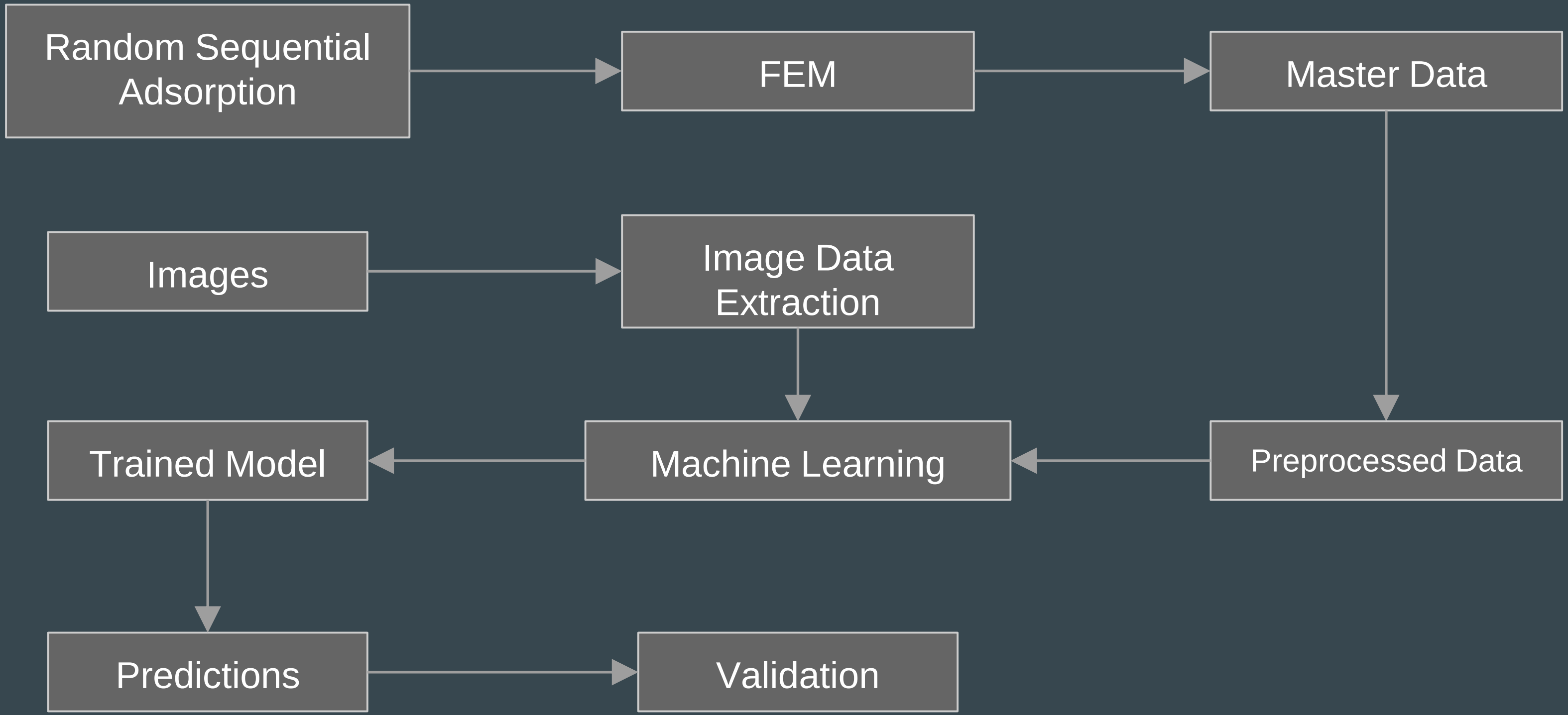


Image Data Extraction

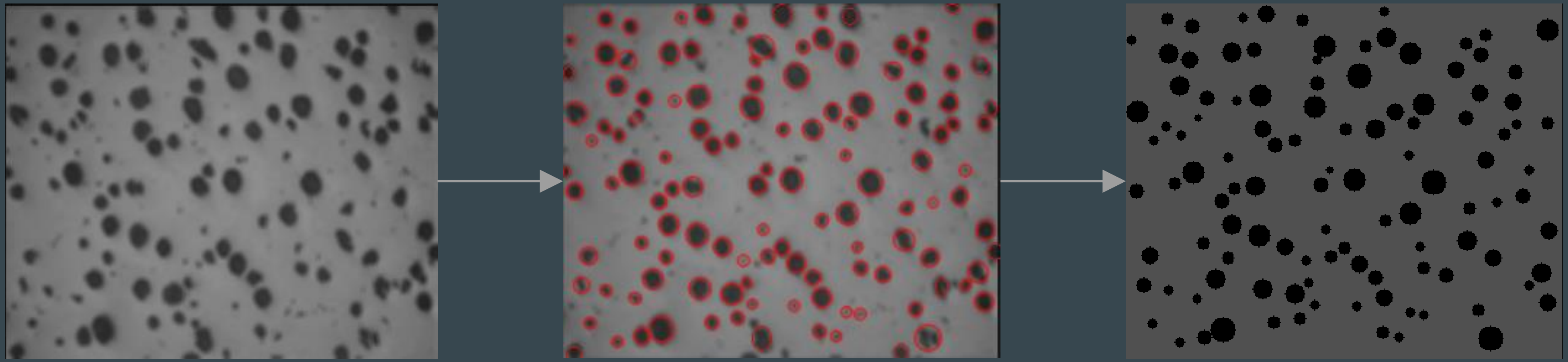


Image Data Extraction

In [25]:
```
im = cv2.imread("1002.BMP", cv2.IMREAD_GRAYSCALE)
im = smothenImage(im)
detector = initialiseBlobDetector()

keypoints = detector.detect(im)
keypointsData = extractKeypointsData(keypoints)
# showDetection(im, keypoints, keypointsData)
# imFinal = createImageCopy(im, keypointsData)
```

In [27]:
```
height, width = im.shape
area = height*width
keypointsData['AreaOfBlobs'] = np.pi*keypointsData['Radius']**2
volumeFraction = keypointsData['AreaOfBlobs'].sum() / area
print 'Volume Fraction of the input Composite image is ' + str(volumeFraction)
```

```
Volume Fraction of the input Composite image is 0.152864484281
```

In [28]:
```
keypointsData
```

Out[28]:

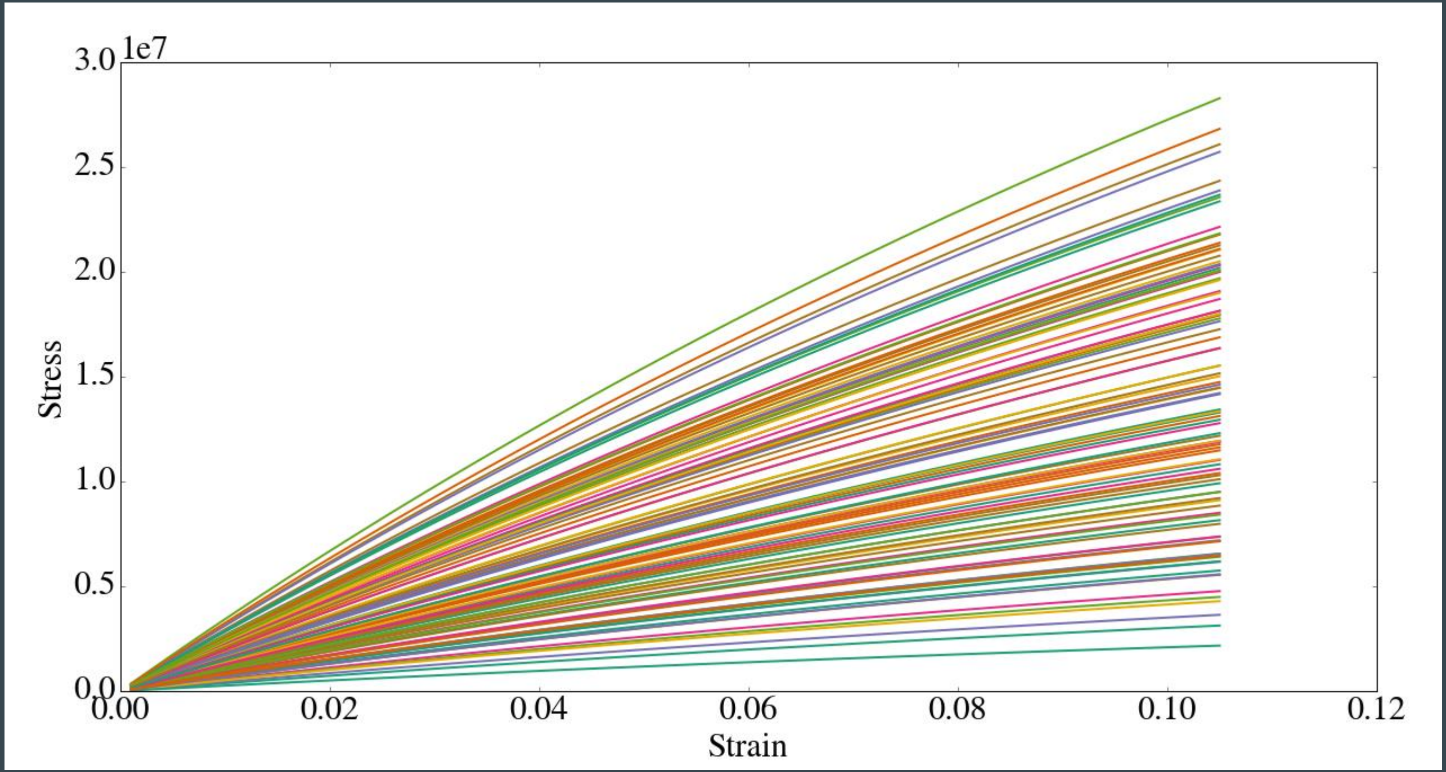
	Diameter	PtX	PtY	Radius	AreaOfBlobs
0	12.836687	63.091553	269.027771	6.418344	129.418330
1	20.303453	78.846146	263.404114	10.151727	323.764859
2	10.625246	284.939880	247.163132	5.312623	88.668196
3	15.425774	340.525360	241.271255	7.712887	186.889021
4	15.390263	341.608276	183.140594	7.695131	186.029553
5	13.618959	320.703003	155.688995	6.809480	145.672554

Data for Constructing Stress-Strain Curve

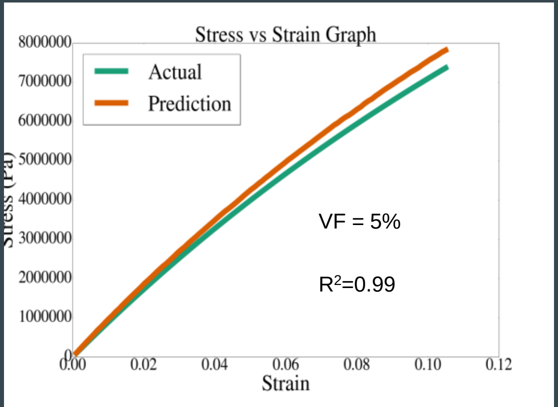
The first data set is created for building the stress-strain curves for various composites.

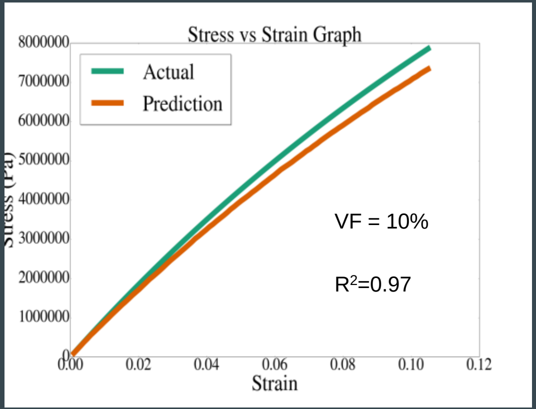
1. For this, the following features are considered:
   a. Youngs Moduli of matrix and fibre
   b. Poisson's Ratios of matrix and fibre
   c. Strain (normally distributed; 10 values considered)
   d. Volume fraction (5%-30%, in increments of 5%)
2. Characteristics of data:
   a. Total size (rows) of data = 60,000
   b. Number of unique materials = 100

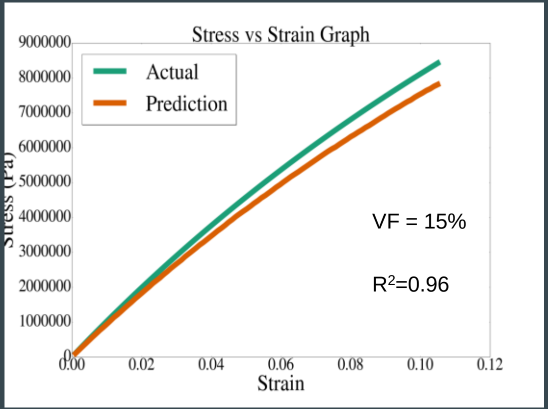
Range of Data Considered



Results: Stress-Strain Curves at Different Volume Fractions





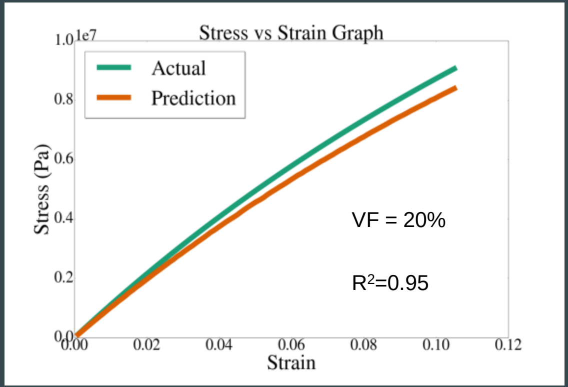


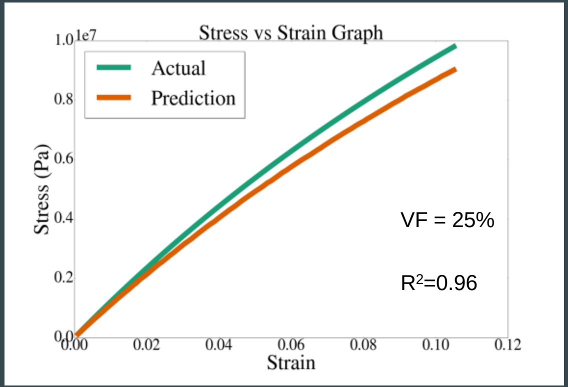
VF: 5%

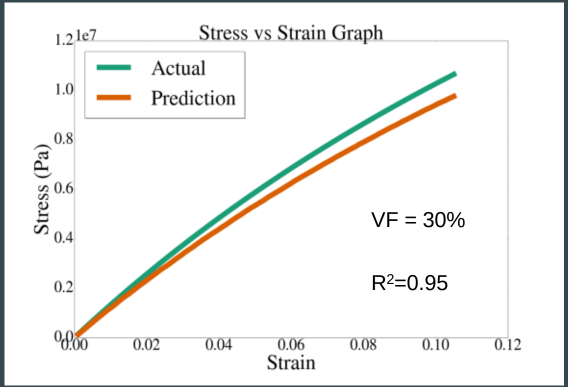
VF:10%

VF:15%

Results: Stress-Strain Curves at Different Volume Fractions







VF:20%

VF:25%

VF:30%

Random Sequential Adsorption Model

To generate a statistically equivalent RVE, the **Random Sequential Adsorption** model was used. This method creates a set of randomly distributed distributed points inside a square region, with the constraint that no pair of points may be closer points inside a square region and no closer than a certain minimum distance.

Steps:

- Setting the values of volume fraction
- Limit the distance between fibres (circles) and between circles and the walls of the unit cell
- Required diameter of circles and their number is determined
- Required arrangement is obtained in a random manner to ensure isotropic nature

Finite Element Method

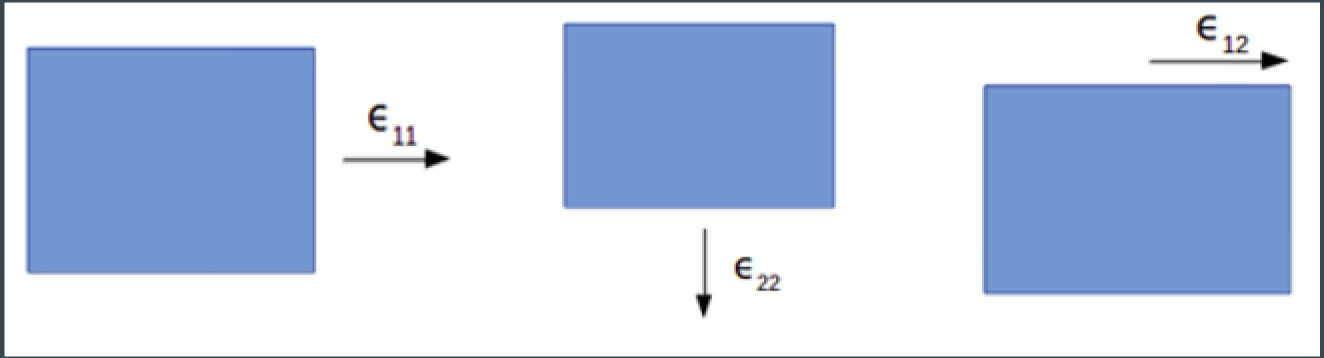
Steps

1. Generate 5 microstructures for each composite for each volume fraction
    a. Volume fraction = {0.3, 0.4, 0.5}
    b. Plane strain (ϵ_{11}, ϵ_{22}, ϵ_{12})
    c. Composite range shown on the following slide
2. Obtain the average stress values
    - When L/d > 20, the difference observed due to spatial arrangement of particles is not significant
    - L = Length of unit cell, d = diameter of particles
3. Obtain tangent moduli (formulae shown later)
4. Feed tangent moduli data to ML model

Description of Generated Data

	Stress (Pa)	Matrix Young's Modulus (Pa)	Matrix Poisson's Ratio	Fibre Young's Modulus (Pa)	Fibre Poisson's Ratio	Strain	Volume Fraction (%)
count	6.00e+04	6.00e+04	6.00e+04	6.00e+04	6.00e+04	6.00e+04	6.00e+04
mean	9.159537e+08	5.9948e+09	0.42476	5.063630e+11	0.320730	0.052192	17.500000
std	6.753535e+08	2.4735e+09	0.01544	2.830782e+11	0.018896	0.030326	8.539197
min	2.672000e+06	1.1500e+09	0.40000	1.030000e+10	0.282000	0.001001	5.000000
25%	3.772325e+08	4.1600e+09	0.41000	2.590000e+11	0.306750	0.026082	10.000000
50%	7.670250e+08	5.8600e+09	0.42400	4.845000e+11	0.322500	0.051775	17.500000
75%	1.322200e+09	8.0975e+09	0.43825	7.527500e+11	0.338000	0.078081	25.000000
max	3.958600e+09	9.9600e+09	0.45000	9.990000e+11	0.350000	0.105000	30.000000

Tangent Moduli Formulae



$$\overline{D_{1111}} = \frac{\partial \overline{\sigma_{11}}}{\partial \overline{\epsilon_{11}}}$$

$$\overline{D_{2222}} = \frac{\partial \overline{\sigma_{22}}}{\partial \overline{\epsilon_{22}}}$$

$$\overline{D_{1212}} = \frac{\partial \overline{\sigma_{12}}}{\partial \overline{\epsilon_{12}}}$$

$$\{\bar{\sigma}\} = \{\bar{D}\}\,\{\bar{\epsilon}\}$$

Machine Learning

Training

1. Features:

   a. Young's Modulus of Matrix (E_m) and Fibre (E_f)

   b. Poisson's Ratio of Matrix (ν_m) and Fibre (ν_f)

   c. Volume Fraction (Φ) - obtained from image or set to {0.3, 0.4, 0.5} during generation from FEM

   d. Tangent Moduli (FEM)

2. Target:
   Tangent Moduli (D_{1111}, D_{2222}, D_{1212})

Machine Learning

3. Algorithms:

   a. XGBoost Regressor (XGB)

   b. Random Forest Regressor (RF)

   c. Ensemble of XGB and RF

3. After obtaining the tangent moduli, apply relevant formulae (given on next page) to get:

   a. Young's Modulus of composite (E_m)

   b. Shear Modulus of composite (D_{1212})

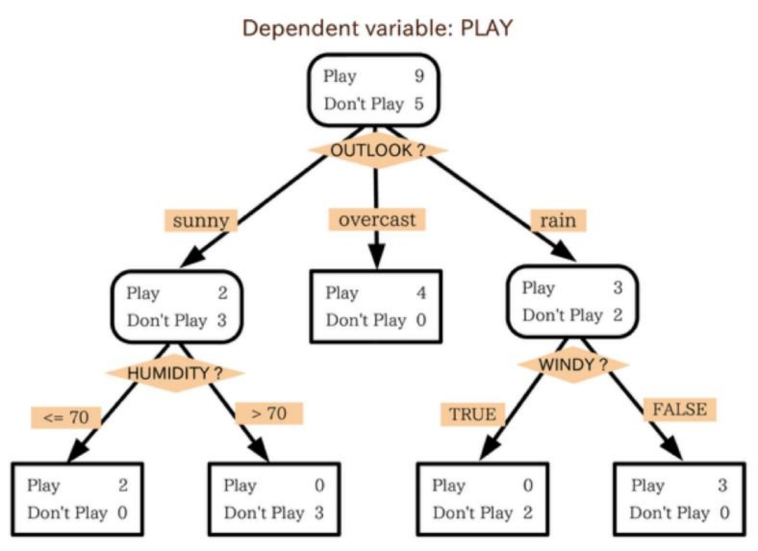
   c. Poisson's ratio of composite (ν_c)

$$x = \frac{2 \times D_{1212}}{D_{1111}}$$

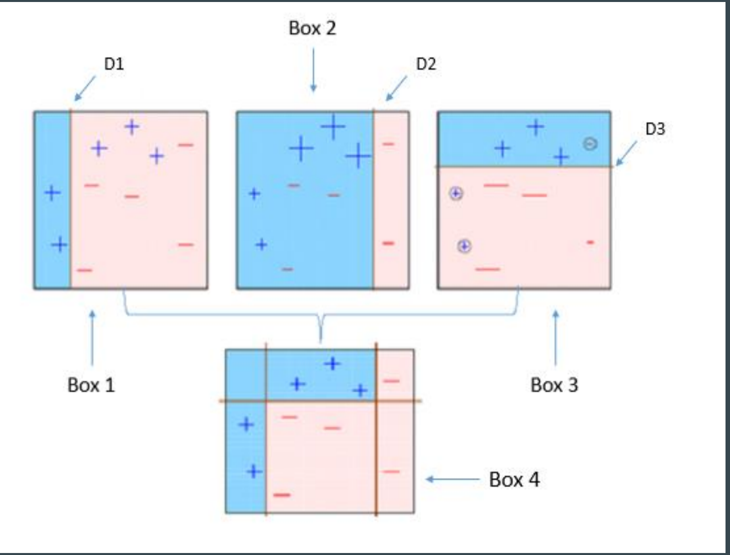
$$\nu_c = \frac{x-1}{x-2}$$

$$E_c = D_{1212} \times 2 \times (1 + \nu_c)$$

Machine Learning Algorithms



Decision Tree



Decision Tree Algorithm (Graphically)

Procedure

- We considered two composites with properties in our predictable range.

    - Glass (Fibre) - Epoxy (Matrix)
        - $E_f = 71$ GPa
        - $\nu_f = 0.22$
        - $E_m = 4$ GPa
        - $\nu_m = 0.35$

    - Boron (Fibre) - Epoxy (Matrix)
        - $E_f = 420$ GPa
        - $\nu_f = 0.2$
        - $E_m = 4$ GPa
        - $\nu_m = 0.35$

Procedure

- Made predictions on 3 different volume fractions
  - Volume Fractions (Φ) = 0.3, 0.4, 0.5
- Inputs - E_m, ν_m, E_f , ν_f , Φ

In [15]:
```
to_predict1.columns = ['E_m','nu_m','E_f','nu_f','phi']
to_predict1
```

Out[15]:

	E_m	nu_m	E_f	nu_f	phi
0	4.000000e+09	0.35	7.100000e+10	0.22	0.3
1	4.000000e+09	0.35	7.100000e+10	0.22	0.4
2	4.000000e+09	0.35	7.100000e+10	0.22	0.5

In [16]:
```
to_predict2.columns = ['E_m','nu_m','E_f','nu_f','phi']
to_predict2
```

Out[16]:

	E_m	nu_m	E_f	nu_f	phi
0	4.000000e+09	0.35	4.200000e+11	0.2	0.3
1	4.000000e+09	0.35	4.200000e+11	0.2	0.4
2	4.000000e+09	0.35	4.200000e+11	0.2	0.5

Procedure

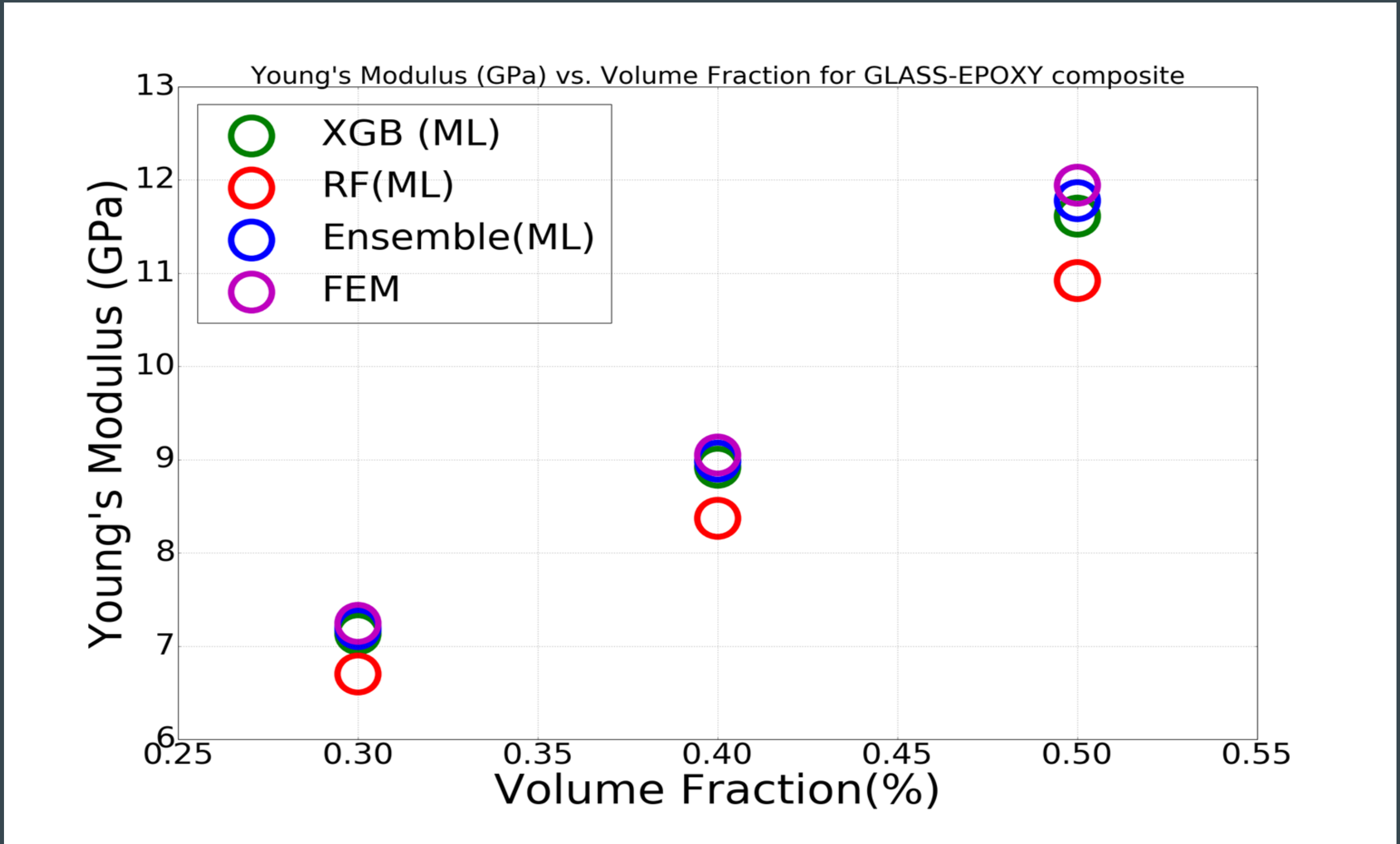
- Predictions
  - Glass-Epoxy

	E	phi
0	7.072853	0.3
1	8.773520	0.4
2	11.664627	0.5

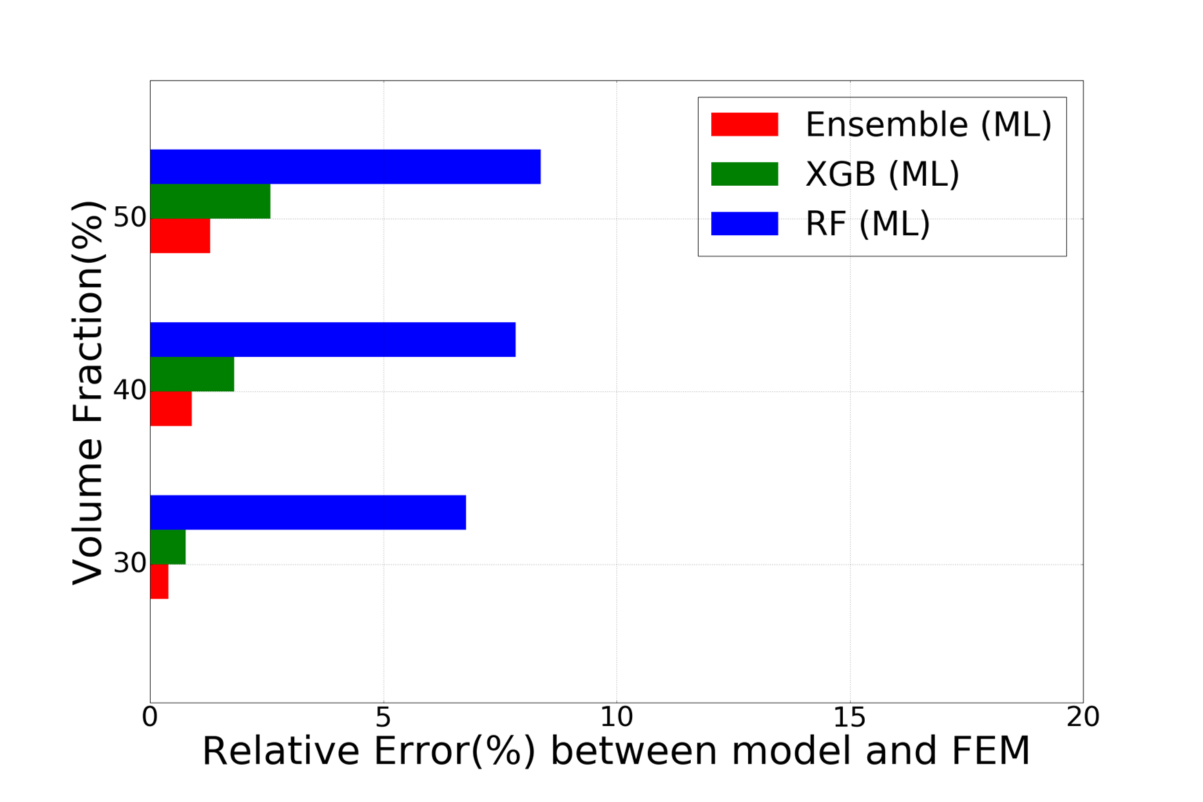
  - Boron-Epoxy

	E	phi
0	7.213498	0.3
1	9.191530	0.4
2	12.933981	0.5

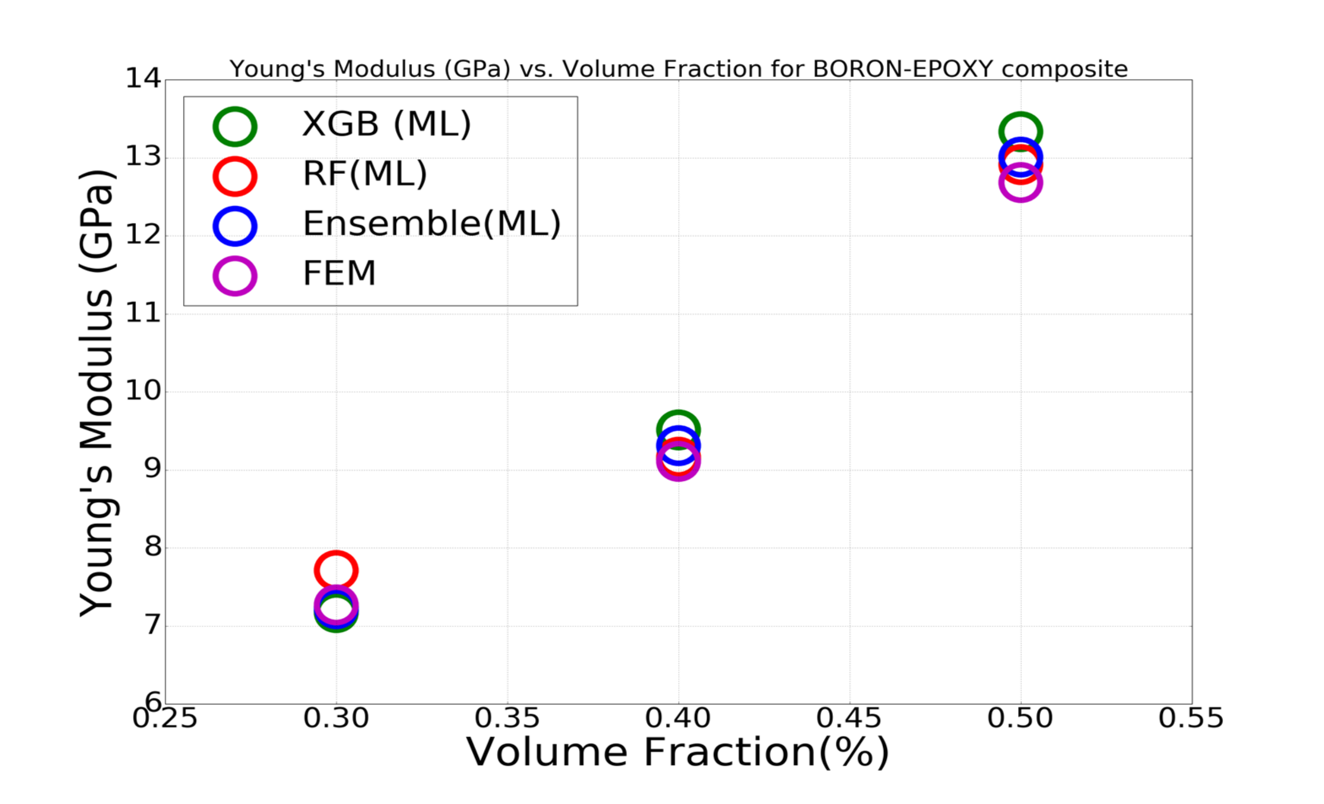
Accuracy Comparison (Young's Modulus)



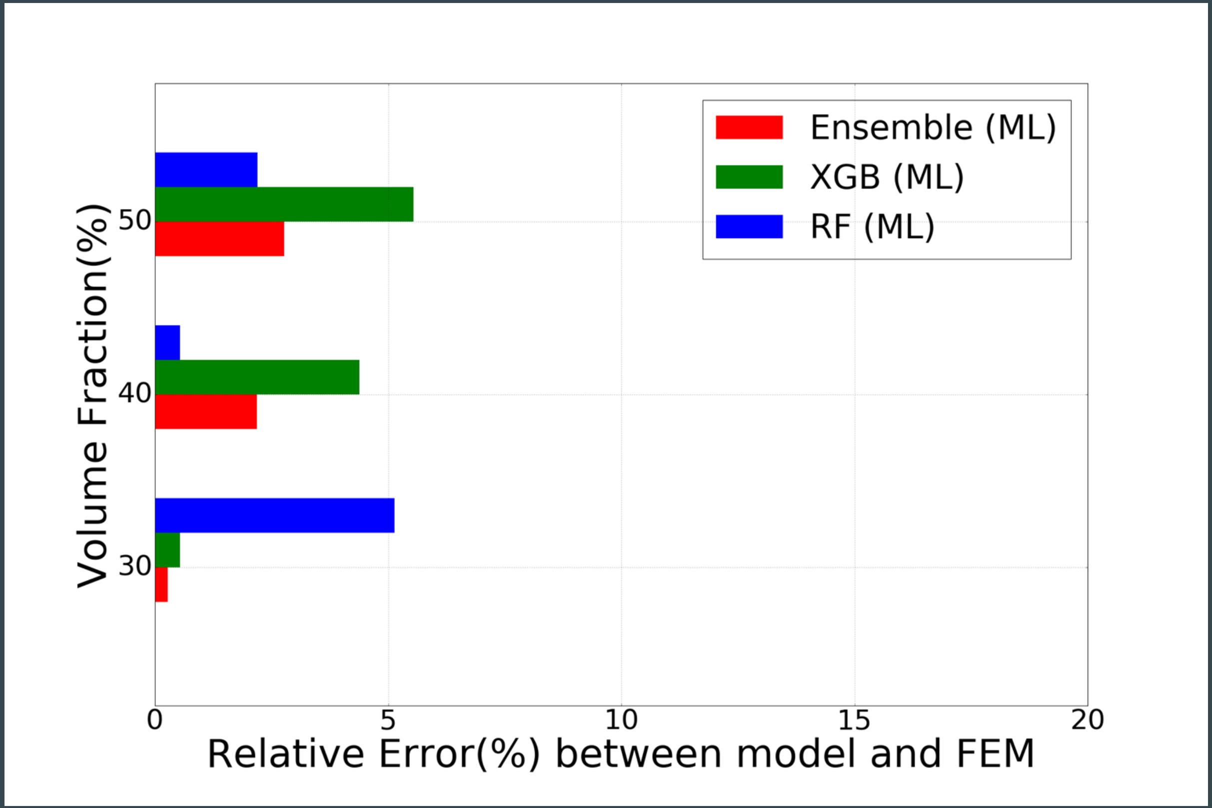
Percentage Error - Glass Epoxy (Young's Modulus)



Accuracy Comparison (Young's Modulus)



Percentage Error - Boron Epoxy (Young's Modulus)



Conclusions: Findings of the Present Work

- A data set comprising nearly **300 different types of materials**, when fed to the Machine Learning model, is **satisfactorily sufficient** in predicting properties of virtually all materials in the range of the data.

- **Ensembles** of several different Machine Learning models tend to **perform better** than more powerful single models in capturing trends in the data. Furthermore, it also helps in reducing overfitting and building a more robust model.

- A Machine Learning approach for **constructing the stress-strain curve** of a new composite material gives **promising results** on different materials with different volume fractions, provided the strain is in the range of the data.

Conclusions: Future Scope

- **Variation in several other properties** of materials like de-bonding of particles/fibres, ductility, and matrix failure (which can be used to calculate toughness and strength) can be introduced.

- A **more comprehensive database** containing information on the manufacturing process of a material, shape, size, etc. can be constructed to enable this data to be used in industry.

- Development of **faster and automated techniques** for generation of composite materials with **high volume fractions**.

- The analysis can be extended to particles/fibres of **different diameters**.

- The analysis can be **extended to 3 dimensions** with the introduction of particles. However, it would be significantly more computationally expensive.


Thank You