Current Progress:

Our project aims to unite and extend the current analytical equations for predicting the thermal conductivity of composite materials using machine learning algorithms. We started the research by learning the basic theories and figured out a method to generate training data using the misoriented ellipsoid inclusion model provided by Ce-Wen Nan *et al.* With the training data, we succeeded in training a reliable machine learning model that has a prediction accuracy of within 10% with the Nan's model for the same material configuration. We attribute this high level of accuracy to the introduction of two unique parameters : the φ (sphericity of the inclusion) and p (the ratio of the two perpendicular dimensions of the inclusion) to describe the shape of the particles.

We concurrently used Comsol, a software that calculates the thermal conductivity based on finite element methods, to verify independently the result from our machine learning model. For the case of the ellipsoid inclusion, the simulation results are quite close to the predicted and analytical results. On this basis, we tested the machines learning model with other particle shapes, such as sphere, cube, core and donuts etc. The results, except for some extreme input values, the machine learning model gives very good prediction with a relative predict error within 10% of the result calculated from finite element.

To conclude, hitherto we are successful in training and testing the model under various situations and cases. We find that the shape of particles does affect the overall conductivity of the composite material. While this effect is relatively small compared to other parameters, our machine learning model can still distinguish the difference with relatively small errors (<10%).

The results and gains heretofore:

So far, we have a systematic method to generate training data based on the various analytical effective medium models. We have used this data to train and run a complex regression model for predicting the thermal conductivity of composite materials. We have introduced two factors: sphericity and *p* in the machine learning training process to describe the shape of the particles that resulted in excellent agreement with the analytical models. We have compared the results from the trained machine learning model with the finite element software and found good agreement for shapes outside the training set with relatively low errors.

Analysis of main problems existing:

Problem#1: The links among effective medium theory, machine learning model and simulation results by finite element method is still obscured.
Solution: By reviewing the current test results and carrying out more tests, we will attempt to formulate the relationship between effective medium theory and machine learning model. In other word, we will try to modify the analytical model based on results from our machine learning model.

Problem#2: The parameter p is not rigorously defined for different particle shapes.
Solution: With the machine learning model we tested different p values for each shape to find which fits the simulation result best. By collecting these potential p values and analyzing them together with the corresponding shape, we may be able to conclude relationship between the p value and shape.

Problem#3: The cases and shapes of particle we currently test with the model is relatively messy and arbitrary e.g. some cases are tested with cube while not with core and donuts.
Solution: Review the verification process to see what tests are still needed and document these testing results.

Main tasks and schedule for the next stage:

Task I : (Dec 2019 to end)
Formulating the relationship between effective medium theory and machine learning model. For different shapes, try to modify the effective medium theory's formula to make it easier to apply for various particle shapes.

Task II : (Dec 2019 to March 2020)
Elucidate the limits of our trained model

Task III : (Dec 2019 to March 2020)
Test with more extreme cases to document and finish a draft for paper submission.