

A Machine Learning Approach for Impact Damage Quantification in Polymer Matrix Composites

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ABSTRACT

Largely due to superior properties compared to traditional materials, the use of polymer matrix composites (PMC) has been expanding in several industries such as aerospace, transportation, defense, and marine. However, the anisotropy and non-homogeneity of these structures contribute to the difficulty in evaluating structural integrity; damage sites can occur at multiple locations and length scales and are hard to track over time. This can lead to unpredictable and expensive failure of a safety-critical structure, thus creating a need for non-destructive evaluation (NDE) techniques which can detect and quantify small-scale damage sites and track their progression. Our research group has improved upon classical microwave techniques to address these needs; utilizing a custom device to move a sample within a resonant cavity and create a spatial map of relative permittivity. We capitalize on the inevitable presence of moisture within the polymer network to detect damage. The differing migration inclinations of absorbed water molecules in a pristine versus a damaged composite alters the respective concentrations of the two chemical states of moisture. The greater concentration of free water molecules residing in the damage sites exhibit highly different relative permittivity when compared to the higher ratio of polymer-bound water molecules in the undamaged areas. Currently, the technique has shown the ability to detect impact damage across a range of damage levels and gravimetric moisture contents but is not able to specifically quantify damage extent with regards to impact energy level.

The applicability of machine learning (ML) to composite materials is substantial, with uses in areas like manufacturing and design, prediction of structural properties, and damage detection. Using traditional NDE techniques in conjunction with supervised or unsupervised ML has been shown to improve the accuracy, reliability, or efficiency of the existing methods. In this work, we explore the use of a combined unsupervised/supervised ML approach to determine a damage boundary and quantification of single-impact specimens. Dry composite specimens were damaged via drop tower to induce one central impact site of 0, 2, or 3 Joules. After moisture exposure,

each specimen underwent dielectric mapping, and spatial permittivity maps were created at a variety of gravimetric moisture contents. An unsupervised K-means clustering algorithm was applied to the dielectric data to segment the levels of damage and define a damage boundary. Subsequently, supervised learning was used to quantify damage using features including but not limited to thickness, moisture content, permittivity values of each cluster, and average distance between points in each cluster. A regression model was trained on several samples with impact energy as the predicted variable. Evaluation was then performed based on prediction accuracy for samples in which the impact energies are not known to the model.

INTRODUCTION

The global composites market was estimated at 89 billion USD in 2019 and continues to grow rapidly with a projected market size of 164 billion USD by 2027 [1]. This is primarily driven by the demand for lightweight materials in a variety of industries, such as aerospace, defense, marine and oil, renewable energy, and automotive [2]–[4]. Polymer matrix composites (PMC) specifically offer a multitude of advantages over traditional materials, like metals. This includes a high strength-to-weight ratio, excellent dielectric properties, improved corrosion resistance, and the ability to tailor laminate design to fit desired mechanical properties. However, this varying degree of anisotropy can lead to complex damage mechanisms when structures are subjected to stressors such as mechanical loading or environmental events [2], [5]. These occurrences cause the formation of nano-scale damage sites throughout the structure, involving rupture mechanisms like matrix cracking and interfacial debonding as the damage grows. The accumulation of these sites can ultimately end in catastrophic failure of a part, especially due to the non-visible nature of damage [5], [6].

Due to this, reliable non-destructive evaluation (NDE) techniques are critical in failure prevention, particularly as the use of PMCs becomes more widespread. Popular methods used in industry currently include tap testing, ultrasound, micro-CT, and thermography, among others [7], [8]. These techniques can detect damage, but generally have difficulty with detection of early-stage or non-visible damage. In pursuit of a technique which can detect and quantify hidden, early-stage damage, our lab has developed a microwave technique that capitalizes on atomistic interactions between water molecules and the matrix in a PMC [9]–[12]. Within a polymer matrix, water exists in two states: ‘bound’ to the network or ‘free’ of external interactions. Under an applied electromagnetic field, bound water cannot rotate, while free water rotates unimpeded, leading to highly different dielectric properties [13]. Bound water has a relative permittivity of about 3, while free water records a relative permittivity closer to 80. The preferential migration of free water to microcracks and voids within the matrix allows the use of moisture as an “imaging agent” to map the damage within a structure. The free water locally elevates the permittivity signature at the damage sites, meaning that a contour plot of permittivity values can be used to identify damage location. We have demonstrated that our NDE technique is highly sensitive to small-scale damage at low levels of moisture [14]–[16]. The technique can reliably detect and locate damage due to impact but has not yet shown the ability to quantify the extent of damage. This is critical to the evaluation process; the information can be used to determine whether a part repair or replacement may be required.

Machine learning algorithms have accelerated the composite NDE and structural health monitoring (SHM) fields by enabling damage detection, localization, classification, quantification, and prediction of remaining part life based on damage features. Two basic approaches of ML include supervised learning and unsupervised learning. The supervised learning technique introduces a labeled dataset to an algorithm for training, and the algorithm internally adjusts parameters to fit the training dataset. It can then be used to classify data into categories (classification) or predict a numerical outcome (regression) [17]. Unsupervised learning uses algorithms to analyze an unlabeled dataset; these models are typically used for clustering, pattern recognition, or dimensionality reduction [18]. In most cases of ML for NDE applications, supervised learning has been used due to the necessity to identify the characteristics at a damaged or undamaged point within a sample [17]. However, we have found that for detection and localization of impact damage in a polymer composite, an unsupervised K-means clustering algorithm used on the raw data collected from our developed dielectric method has performed well. While a promising improvement to the dielectric NDE method, this algorithm alone cannot provide information about the extent of damage. To address this, we propose utilizing a supervised algorithm on the clustered data to predict the energy level of a single impact event.

The use of supervised learning algorithms for damage classification or prediction has been prevalent in literature. Amali and Hughes [19] detail work in which they use a computer program to detect changes in acoustic response during tap testing. A 3-layer feed-forward neural network was used to classify the state of a sample as damaged or undamaged; the algorithm correctly identified damage state for seven of eight inputs. Farooq et. al used support vector machines (SVM) and artificial neural networks (ANN) to detect and identify damage in smart structures [20]. Strain data collected via finite element analysis for damaged and healthy laminates was used to train the algorithms as classifiers; both algorithms showed high accuracy in binary classification. Dabetwar et. al used Lamb wave signals collected by NASA and the features acquired from the signals were used to train and test four supervised machine learning algorithms [21]. Performance indicators showed that for damage classification, SVM had difficulty classifying into three classes, while k-nearest neighbors (KNN), decision tree, and random forest performed better. To quantify damage rather than solely classify a location as damaged or undamaged, regression models show promise. Datta et. al used least square support vector regression (LS-SVR) to localize impact damage and estimate severity in carbon fiber reinforced polymer (CFRP) structures [22]. Three models were trained based on features from data collected via Fiber Bragg grating sensors; the respective models were used to predict (i) impact energy, (ii) x-coordinates of the impact location, and (iii) y-coordinates of the impact location. The proposed LS-SVR algorithm performed better than four differing algorithms in literature, one of which was another LS-SVR proposed by Xu also for damage localization and quantitative assessment [23].

The use of machine learning to improve NDE techniques for damage detection, localization, and assessment in composites is well documented. In this work, we have applied a support vector regression (SVR) algorithm to dielectric data that has first been processed using an unsupervised k-means clustering algorithm.

EXPERIMENTAL DATA COLLECTION

Specimen Preparation

Test samples were created using a prepreg consisting of a Hexcel F161 epoxy resin and a crowfoot weave glass fabric, Style 120. Twenty-two plies of prepreg with dimensions of 305 x 178 mm were laid up and cured in a hot press at 772 kPa. The plies were heated under pressure at a steady rate of 10°C/minute until they reached 180°C and maintained for two hours under these conditions. Afterwards, it was cooled to room temperature at an approximate rate of 2°C/minute. Test specimens were cut from the larger laminate using a diamond saw to size 100 x 55 mm. Laminate properties were obtained via resin burn-off in accordance with ASTM D3171 [24]. Smaller specimens were placed in a high-temperature furnace maintained at 800°C until the entirety of the matrix was removed. Estimated fiber, matrix, and void contents obtained via weights pre and post burn-off are given in Table 1.

TABLE I. EPOXY/GLASS LAMINATE PROPERTIES.

Property	Mean (%)	Standard Deviation (%)
Fiber Volume Fraction	51.36	0.72
Matrix Volume Fraction	43.32	0.63
Void Volume Fraction	5.32	0.58

The test specimens were dried in a vacuum oven at 65°C until a dry stable weight was achieved in accordance with ASTM D5229 [25]. Once dry, each specimen was subjected to a low-velocity, out-of-plane impact event via drop tower. A hemispherical striker tip of 9 mm radius was attached to a crosshead and dropped at the appropriate height to induce barely visible damage at the approximate center of each sample. Four specimens were impacted at an energy of 2 Joules and another four at 3 Joules, while three specimens remained unimpacted as the representative control group of 0 Joule damage. The amount of induced damage was controlled by adjusting the drop height of the crosshead.

Moisture Contamination

After specimen drying and impact, weight data was recorded prior to beginning moisture uptake. The samples were then immersed in a deionized water bath to

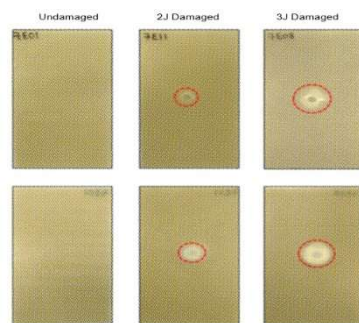


Figure 1. Images of front (top) and back (bottom) of samples at 0, 2, and 3J damage.

accelerate moisture absorption. The bath was maintained at 25°C. Specimen weights were recorded periodically using a Mettler-Toledo high-precision analytical balance, and moisture content is obtained by referencing the previously recorded dry weight.

Dielectric Data Acquisition

Dielectric data for each sample was collected at several moisture levels between 0.05 and 0.6% gravimetric moisture content. These are acquired using a split-post dielectric resonator (SPDR) connected to a vector network analyzer (VNA). This enables the measurement of bulk relative permittivity and tracking of small changes on the order of 10^{-3} with a high accuracy of 0.3% uncertainty [26]. Before taking measurements, the system was calibrated via adjustment of the scattering parameters S11, S22, and S21, which represent the magnitude of the reflected signal at port 1, port 2, and the transmitted signal from port 1 to port 2, respectively. Prior to specimen insertion into the cavity, the resonant frequency of the empty resonator is recorded. The shift in frequency is then recorded upon sample insertion. These values along with sample thickness, are used to calculate the real part of relative permittivity. This formula is shown below in Eq. 1 [26].

$$\epsilon'_r = 1 + \frac{f_0 - f_s}{h f_0 K_\epsilon(\epsilon'_r, h)} \quad (1)$$

where

- f_0 is resonant frequency of empty SPDR
- f_s is resonant frequency with the dielectric specimen inserted
- h is sample thickness
- K_ϵ is a function of ϵ'_r and h , documented in a table unique to each SPDR and provided by the manufacturer

Spatial relative permittivity maps are created using a novel mapping device developed by our lab. The device primarily consists of NEMA-17 stepper motors, linear screw actuators, and A4988 motor drivers controlled by an Arduino MEGA 2560 board coupled with a MATLAB script. The specimen is held within the cavity using a 3D-printed holder coupled with a spring. Based on inputs of x and y step sizes, the motors move a specified distance, subsequently moving the specimen within the cavity. The VNA is then triggered, and data is stored in an excel sheet. This process is repeated until dielectric measurements have been completed to make a spatial map of resolution based on given step size. An image of the device with a specimen inserted is shown in Figure 2.

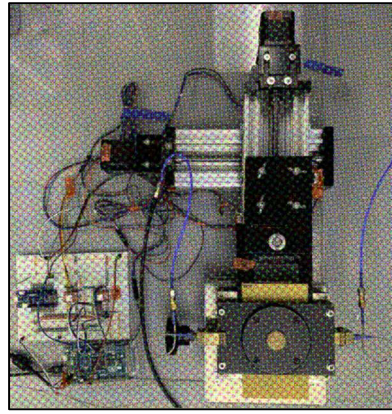


Figure 2. Image of damage mapping device with specimen inserted.

MACHINE LEARNING ALGORITHMS

Unsupervised K-means Clustering Algorithm for Damage Location

To detect damage and determine location within the sample, an unsupervised k-means clustering algorithm was applied to the raw data collected from the dielectric scans at each moisture content. The k-means algorithm is capable of detecting patterns in unlabeled data and grouping them into heterogeneous sets, called clusters. K-means clustering is an exclusive clustering algorithm, meaning that data points can only belong to one cluster. To determine which data points should belong to which cluster, the algorithm runs as follows: an original center is defined for each cluster “k” decided a-priori. Each point is assigned to the nearest cluster center. These centers are then recalculated iteratively until the center points are unchanged with continuing iterations. Simultaneously, the algorithm aims to minimize an error function defined as the distance between data points and their assigned cluster centers [27], [28]. A challenge in this approach is the requirement to define the number of clusters “k” prior to performing clustering. There are two primary methods to determine the optimal number of clusters to segment the data: the elbow method and the silhouette method. In this case, we have used the elbow method. This plots the cluster inertia against the number of clusters used to group the data. Inertia is the sum of squared distance from each data point to its assigned cluster center. At a higher number of clusters, inertia will decrease because points are inherently closer to a cluster center but increasing the number of clusters can lead to overfitting the data. Thus, the number of clusters at the “elbow” of the curve, or inflection point, is considered to be the optimal number of clusters [29].

During collection, the dielectric data is stored as an array of three values: relative permittivity, loss tangent, and bandwidth. For each scan, a dry baseline scan of the equivalent sample was subtracted from the data to eliminate variation due to thickness effects. The data was scaled in Python using a ‘MinMaxScaler’ available in the sklearn.preprocessing module to standardize the vectors to values between 0 and 1.

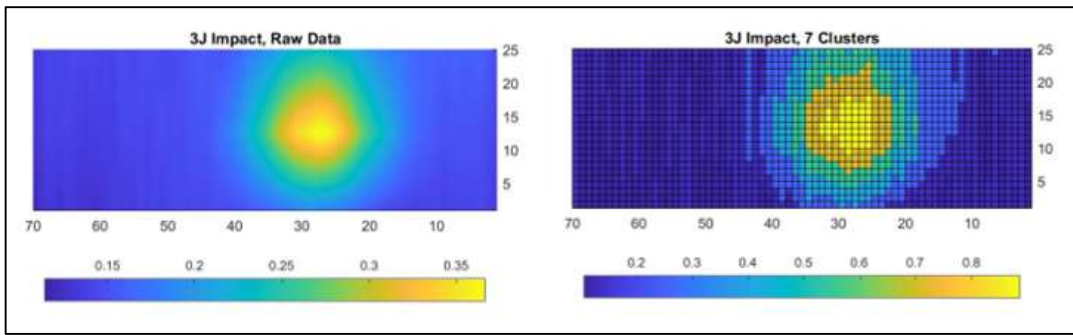


Figure 3. Spatial relative permittivity plot before clustering (left) and after clustering (right).

For each sample, the elbow method was applied to determine optimal number of clusters, and the k-means algorithm was applied. Once the clusters were obtained, the data could be replotted respective to their location on the sample. Examples of the resulting damage before and after clustering is applied is shown in Figure 3. The z-values for the raw data map are subtracted relative permittivity values, while the z-values for the clustered map are a scaled ‘damage indicator’.

Supervised Regression Algorithm for Damage Quantification

Support vector machines (SVM) is a highly utilized supervised machine learning algorithm originally developed for binary classification problems. The main idea of SVM is that it creates a classifier to best separate linear or non-linear training data into classes based on their features. SVM is particularly useful because it can handle data of higher dimensions. With data of one, two, or three dimensions, the classifier is a point, line, or plane, respectively. When the data is in four or more dimensions, the support vector classifier is a hyperplane. SVM constructs one or more hyperplanes in a high dimensional space; for classification, the planes are determined such that they have the largest distance between training data points of any class. The larger the margin between classes, the lower the model error [30].

Support vector regression (SVR) was developed as an extension of SVM and is useful to analyze the relationship between a dependent variable and one or more predictor variables, otherwise known as features. Rather than outputting a classification label, this algorithm can provide a quantitative function estimation based on the derived relationship between variables. For regression, the determination of optimal hyperplanes differs slightly from classification. Rather than determine hyperplanes which separate training samples, an ϵ -insensitive loss function is used to determine a hyperplane where the predicted values of all training data will deviate at most ϵ from their actual values [31].

Kernel functions enable the support vector regression and classification algorithms to systematically find hyperplanes in higher dimensions. These functions transform the input data into a higher-dimensional space known as a “kernel space” [31]. Polynomial and radial basis function (RBF) kernels are common to perform SVR on non-linear data. The RBF kernel is highly effective when the relationships between features and response variables are not well known. This kernel functions similarly to the supervised classification algorithm k-nearest neighbors, which classifies test data based on its distance from specified training samples [32]. Based on user-inputted

parameters, the RBF kernel behaves as a weighted nearest neighbor model; closer observations have more influence over how new observations are predicted. Because of the success in using unsupervised k-means clustering to qualitatively analyze the data, we decided to use the RBF kernel (Eq. 2) for the SVR algorithm. The function is used to determine how much influence each observation in the training dataset has on predicting new observations [33]. RBF kernel parameter is σ , and $\|x - x_i\|^2$ is the Euclidean distance between two observations.

$$K(x, x_i) = \exp\left(-\frac{1}{\sigma} * \|x - x_i\|^2\right) \quad (2)$$

Relevant model parameters for implementation of SVR with the RBF kernel in Python are regularization parameter C , the error sensitivity parameter ϵ , and an RBF parameter γ , which is inversely proportional to the RBF parameter in Eq. 2.

FEATURE SELECTION

For a supervised machine learning algorithm to be effective, the selection of features is highly important. Based on previous experiments, we have observed that thickness of the sample and moisture content can affect the dielectric properties. Thus, those were the first two features chosen. To best capture the qualitative features of the clustered map, quantitative features were also calculated from the clustered data. For each cluster, features consisted of relative permittivity, maximum distance between two points, average distance between points, and total number of data points in the cluster. The loss tangent and bandwidth values for the clusters with most and least damage were also included. Thus, a sample consisting of seven clusters had 34 unique features. Because of the highly differing feature values, the ‘MinMaxScaler’ function (as described in the k-means algorithm section) was used to scale the features between 0 and 1 prior to applying the regression model.

RESULTS AND DISCUSSION

The SVR-RBF algorithm was implemented using various scikit learn modules in Python. Feature vectors for 160 unique sample observations were split into training and testing sets of 60/40 percent of the overall data respectively. Relevant model parameters C , ϵ , and γ were chosen via the GridSearchCV function available in the sklearn.model_selection module. This completed an exhaustive search over specified parameter values and evaluated the model efficiency for every combination. The chosen parameter values are found in Table 2. The optimal RBF parameter was determined to be the default function value, which is 1 divided by the number of features per sample.

TABLE II: MODEL PARAMETER VALUES.

Parameter	Value
C	100
ϵ	0.05
γ	0.029

Monte Carlo cross validation was used to ensure reasonable model repeatability; 10 iterations of random sampling were completed. The model was evaluated using metrics R^2 score and mean squared error (MSE). The R^2 score is representative of the proportion of dependent variable variance that is influenced by the sample features. The best possible score is 1.0, so a value close to that indicates a good model fit. It also indicates how well new observations would be predicted using the model. Mean square error is a measure of the error between the actual and predicted values of the dependent variable; a value of 0 would be perfect. The table below shows the metrics for each iteration and the average score for each metric.

TABLE III. MODEL METRICS FOR EACH ALGORITHM ITERATION.

Iteration	R^2 score	MSE
1	0.8906	0.1043
2	0.8509	0.1604
3	0.8515	0.1604
4	0.9381	0.0641
5	0.8381	0.1655
6	0.8645	0.1144
7	0.8410	0.1478
8	0.8660	0.1621
9	0.8964	0.1262
10	0.9124	0.0889
AVERAGE	0.8750	0.1294

The model efficacy can be visualized by plotting several of the predicted impact energy values as well as the actual values. Fig 4. depicts a few of the test data observations from iteration one. At each value on the x-axis, there is an orange point for the predicted impact energy of the sample and a blue point for the actual impact energy. It is noted that for sample 8, the actual energy and the predicted energy are so close in value that the actual energy point is covered by the predicted energy point.

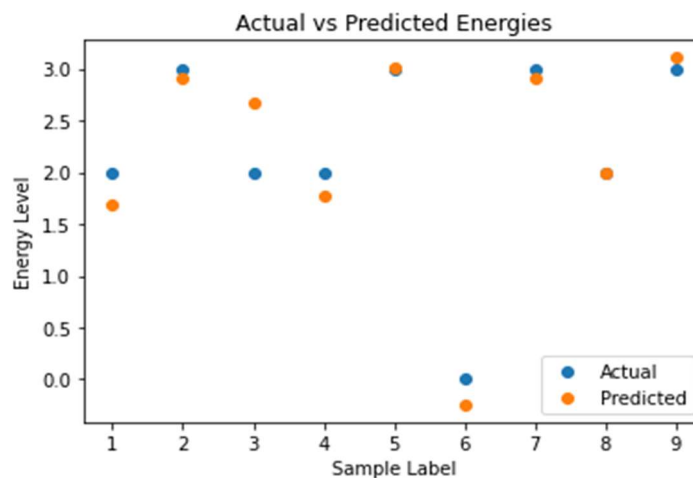


Figure 4. Scatterplot of test observations with model predicted value and actual response value.

It is clear from both the visual representation of the model predictions and the regression metrics that the SVR-RBF does a reasonably good job of impact energy

prediction, with some room for improvement. The average R^2 value is 0.875, which indicates a fairly good model fit. This is promising for the use of regression to supplement the dielectric technique and enable damage assessment and prediction of a structure with non-visible damage. However, it is prudent to consider potential limitations of the predictions. Firstly, both metrics are highly dependent on the dataset. Considering the dataset only included data from one experiment, the model may be affected greatly when data from other experiments, even of the same material system, is introduced. Another consideration is that the number of tested values of impact energy are low. Introducing observations with impact energies of 4, 5, 6 J (etc.) would provide more insight into how well the model can differentiate between marginally differing damage profiles. From the knowledge we have gained through previous experiments, we know the 0 J (undamaged) scans are significantly different from any damaged scans. Thus, this model is likely improved by the inclusion of the 0 J observations. To test this theory, the model was trained and tested on the dataset without any of the 0 J observations. The R^2 score decreased to about 0.7, supporting this idea. To gain a better understanding of the efficacy of the SVR algorithm for damage prediction, sample observations of more variation will need to be added to the dataset.

Another shortcoming of the model is found in the required features. The data used for k-means clustering has been normalized using “dry subtraction”, meaning that a dry baseline scan of the equivalent sample was subtracted prior to ML. In previous experiments, we have found this to be a requirement to obtain meaningful results. In practice, obtaining a dry scan of a structure would be extremely difficult, if not impossible. Hence, in future iterations of this model, both the dry subtracted data and the raw data will be tested to try and eliminate this necessity. Additionally, the inclusion of moisture content as a feature is not ideal, as it is a difficult attribute to obtain for an in-service structure. Moving forward, models will be trained and tested without gravimetric moisture content as a feature to improve the practicality of the technique.

CONCLUSION

A combined supervised/unsupervised machine learning approach was used to estimate the energy associated with impact of single-impact composite specimens. Woven fiberglass samples were impacted and subjected to moisture contamination via immersion in a water bath. Dielectric data was collected at varying intervals of moisture increase using a custom damage mapping device. The data from each scan was clustered using an unsupervised k-means clustering algorithm. Relevant features were extracted from the clustered data, including but not limited to permittivity of each cluster, average distance of points within each cluster, and total number of points in each cluster. These, along with other sample features, were associated with individual observations and these observations were used to train a supervised support vector regression model using a radial basis function kernel to predict impact energy associated with each sample. The model was evaluated using metrics of R^2 score and mean squared error, which had average values of 0.875 and 0.1294, respectively. These values indicated good model fit and response variable prediction.

Potential model pitfalls were discussed. To address these, future work will test the model performance (i) using clustered data without prior dry subtraction, (ii) removing moisture content as a feature, and (iii) adding observations with more

variation in the response variable. To understand the effect of clustering on the model, SVR will also be used directly on the raw data rather than computing features based on clustering. Proceeding with the understanding that the model metrics are affected by dataset size, we are cautiously optimistic. Supplementing the dielectric technique with the ability to estimate damage extent of an unknown scan is exceedingly valuable, especially for use on safety-critical structures. Ultimately, the aim is to create a model trained on several composite material systems at many more damage levels, thus creating a comprehensive model for use on any relevant composite structure.

ACKNOWLEDGEMENTS

This material is based upon work partially supported by the National Science Foundation under Grant No. CMMI-175482.

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