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Implementation of artificial intelligence in the prediction of the elastic characteristics of bio-loaded polypropylene with bamboo fibers

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ABSTRACT

Artificial intelligence is the current trend in the world, which has taken the opportunity to advance in all its fields, particularly in scientific research. In materials engineering, the results obtained from classic methods such as experimentation, homogenization methods, or finite element methods have become input and validation elements for intelligent models to obtain more effective results in an optimal time frame. In this article, we discuss the use of artificial neural networks to determine the mechanical properties of biocomposites, which are the subject of much research due to the advantages they represent. The properties of these complex materials depend on various parameters, such as the behavior of the constituent materials, the percentage of the mixture, and the manufacturing process. In this work, our goal is to predict how polypropylene behaves elastically when reinforced with 15% various natural fillers. and we will study the impact of bamboo on polypropylene to test and validate our model. By exploiting the results of the Mori-Tanaka model, we were able to generate our dataset, with which we feed our feedforward backpropagation neural network and demonstrate that our biocomposite gained in terms of stiffness, marked by an increase in Young's modulus to 550.3 MPa, with better performance validation and a very good regression coefficient.

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1. INTRODUCTION

Bio-composites, also known as innovative materials, are increasingly attracting the attention of contemporary researchers due to the numerous advantages they offer. Their growing popularity across various sectors stems from their ability to provide superior properties compared to their individual constituents, as well as their environmentally friendly nature, in line with the principles of sustainable development. Despite their differences, industries such as automotive, aerospace, food processing, textiles, and others are converging towards the use of bio-composites in their products. As a result, understanding the mechanical properties of eco-composites has become an important area of study, particularly in the context of this research. These properties are defined by various parameters and criteria, such as component characteristics, manufacturing processes, and the percentages of matrix and reinforcement mixtures, among others [1]. Selecting the appropriate bio-composite that meets precise specifications requires a deep understanding of its properties to ensure its proper application. Classical methods widely used by researchers, such as experimentation, homogenization, and finite element analysis, have provided useful information but are inherently limited compared to modern technologies. The homogenization method provides macroscopic estimations of bio-composite properties, while the finite element method relies on simple representative volumes [2]. However, the mechanical properties of bio-composites are influenced by numerous parameters and exhibit highly complex microstructures.

In this study, we focus on the use of artificial intelligence to address the challenges and constraints associated with determining the properties of new materials, particularly bio-composites, as mentioned earlier. Specifically, we use artificial neural networks to predict how polypropylene behaves elastically when reinforced with 15% various natural fillers. By employing a feed-forward backpropagation algorithm, we train our network using the dataset generated by the Mori-Tanaka homogenization method to test and validate our results. The analysis of these results demonstrates the reliability of the chosen artificial model and highlights the adaptability and efficiency of artificial neural networks in solving complex problems. Additionally, our findings underscore the effectiveness of bamboo as a reinforcement, as evidenced by the significant improvement in the rigidity of polypropylene when loaded with this natural fiber compared to pure polypropylene.

2. MATERIALS AND METHODS

2.1. Materials

2.1.1. Polypropylene

With an annual world production exceeding 10 million tons, polypropylene is ranked among the most widely used polymers in various fields. It is characterized by low density, good flexural strength, and compatibility with bio-fillers. It is also recyclable, inexpensive, and versatile [3]. This is why researchers consider it a good candidate as a matrix to study and model the properties of biocomposites. The use of 85% of this isotactic plastic reinforced by natural fibers is the theme of this study. Table 1 and Figure 1 respectively represent the mechanical characteristics and chemical structure of polypropylene.

Table 1. Mechanical and physical properties of polypropylene [4]

Properties	Values	Units
Specific heats, Cp	3100	J/Kg°C
Poisson's ratio,	0.42	
Elastic modulus, E	1034	MPa
Melt density,	0.7751	g/Cm^3
Thermal conductivity, K	0.17	W/m°C

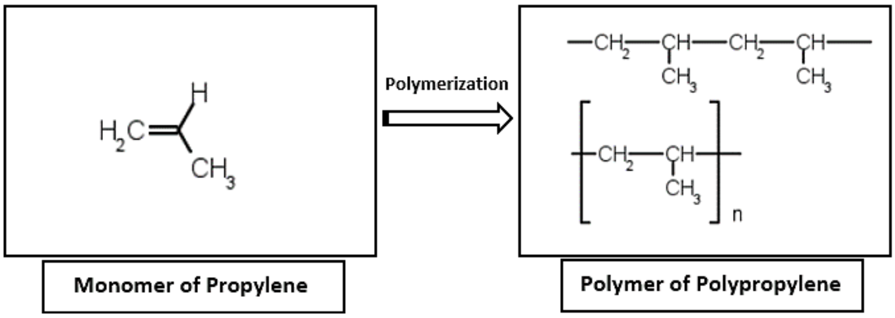

Figure 1. Polypropylene structure [5]

2.1.2. Bamboo fibers

Bamboo fibers are gaining attention from researchers due to the benefits of this uncommonly used material. Bamboo is a renewable and fully recyclable material that has a cylindrical shape, is hollow, and is separated by knots [6]. It is characterized by great rigidity and flexibility. Its growth is very fast, around 20 cm per day and 20 m in 6 months. It matures in 4 years but can be exploited after just one year of growth [7]. Bio-composites from bamboo fibers are mainly used in the construction field, such as supports, and in the automotive sector for veneers or parts such as steering wheels. Figure 2 shows a sample of different breeds of bamboo.

Figure 2. A sample of different bamboo [8]

More than 1,200 bamboo species have been identified worldwide and each species has its mechanical properties. This difference is caused by the growth medium of the bamboo, its geometric shape (diameter of the cylinder, the hollow ...), and others. The process of extracting fibers begins with choosing clean stems that do not contain mold or dry portions. From the 35 cm long sections obtained by cutting between the bamboo knots, the fibers are manually extracted and boiled in water for 5 hours and then dried at 100 °C in air [7]. Figure 3 shows the steps followed to obtain bamboo fibers.

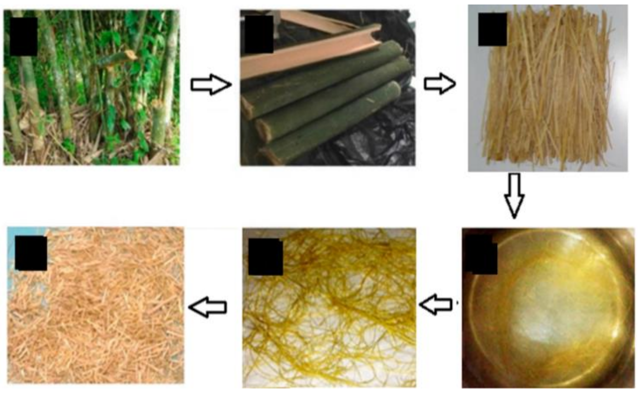

Figure 3. The steps followed to have the fibers begin with choosing the agreed bamboo plant, cutting the sections, then extracting the fibers. The fibers are then boiled, then dried [7]

2.1.3. Composite processing

To determine the mechanical characteristics of our new material and to study the effect of bamboo fibers on polypropylene, these two components were mixed at 180 °C in an internal mixer (HaakeRheomix), and for 10 minutes at a speed of 50 rpm. The rate of natural fibers was set at 15%, to then grind and dry the fiber/PP mixtures. the biocomposite was molded in an injection machine at 200 °C (Krauss Maffei KM50 - 180 CX) [7].

2.2. Methods

Several factors can influence the determination of the mechanical characteristics of biocomposites, yet even if we work under the same conditions, the methods used to calculate the properties of these new materials, do not necessarily give the same results. Each method uses and is based on theorems and assumptions very different from the others, this is what causes different outputs; however, research has been able to show that this difference is approximate. Between experiment, homogenization, and finite element methods there is a certain degree of error, and this is what makes the result even more relative. And the difference is in the precision and also in the calculation time. Smart solutions have come to close this gap and deliver more accurate results in minimum time. In this work, we will use the homogenization method and more precisely the Mori Tanaka model to determine the elastic behavior of polypropylene loaded with natural fibers. Using the results of this model, we will build a dataset from which we will feed an artificial neural network to predict the elasticity of the biocomposite studied.

2.2.1. Dataset/Mori Tanaka's model

Using the Mori Tanaka model in Figure 4, we calculate the modulus of elasticity of the different biocomposites. By introducing Young's modulus of the polypropylene and that of the different bio fillers, we have as an output of this model the bio composites' Young's modulus. As a result, we were able to construct a dataset in the form of a numerical table containing the different values of the inputs and outputs of the model chosen. Mori Tanaka model is one form of the Eshelby solution [9].

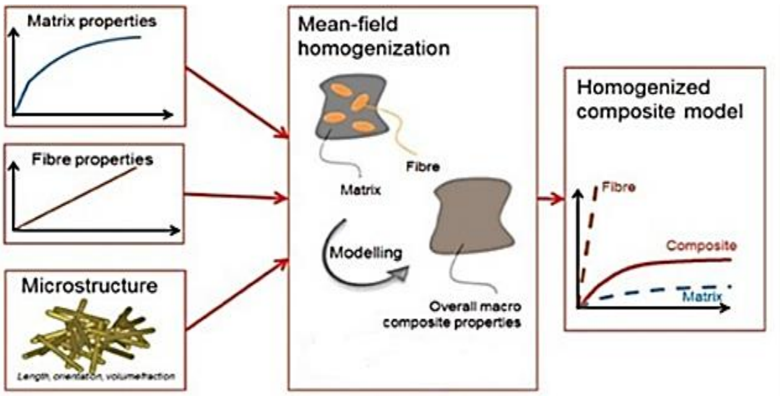

Figure 4. Mean field homogenization method [5]

2.2.3. Artificial neural network

Modeling a regression neural network requires several elements to be defined, such as the objectives of this purpose, the dataset, the target, and others. As explained in the previous section 2.2.1, we used the Maritanaka method to construct our dataset. This dataset will serve as input data in our artificial neural network. In this article, we aim to predict the elastic behavior of biocomposites, specifically the elasticity of polypropylene when it is loaded with 15% biocharge [10]. Therefore, a preliminary analysis of the input elements was conducted in this regard to define the characteristics of the model to be studied. The dataset derived from Mori Tanaka's model exists in digital format, indicating that convolutional neural networks (CNNs), which are designed for image processing [11], are not applicable. Instead, regression neural networks (RNNs) will be employed. RNNs operate by preserving a layer's output and feeding it back to the input layer to generate the layer's output. They consist of layers that allow information processing in both forward and backward directions, as depicted in Figure 5.

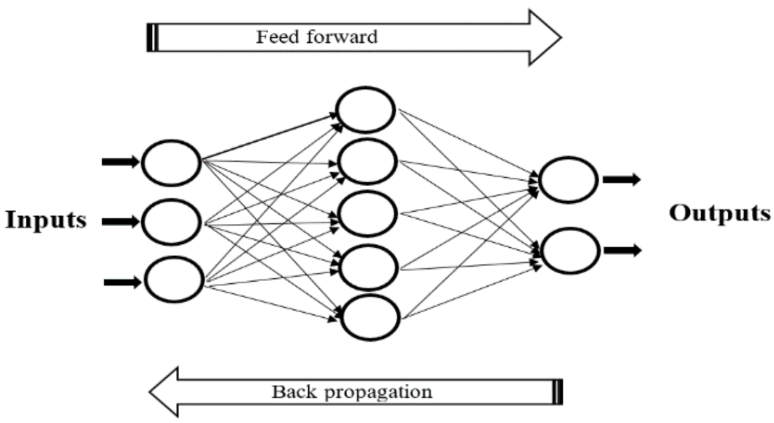

Figure 5. Operating principle of feed-forward backpropagation [12]

Feed-forward backpropagation (FFBP) is the most common and widely used architecture in prediction based on a digital dataset. It has proven to be efficient and has given better results in diabetes prediction, compared to other back propagation architectures [13], especially when it is trained with the Leverbeg-Marquart (LM) algorithm. The LM algorithm represents the most efficient method to accurately train the FFBP [14]. Therefore, and since we are dealing with a non-linear regression problem, the network chosen is the FFBP trained by the LM.

The chosen network then consists of three layers, its topology is in this form 2-h-1. The number 2 represents neurons in the input layer. Number 1 means that we have a single neuron in output. As for the hidden layer (h), we tested it using several neurons ranging from 3 to 20. As a result of the test, we deduced that the most optimal number of neurons that has the maximum performance is 15, hence the topology of our network 2-h (15)-1 as shown by the architecture in Figure 6.

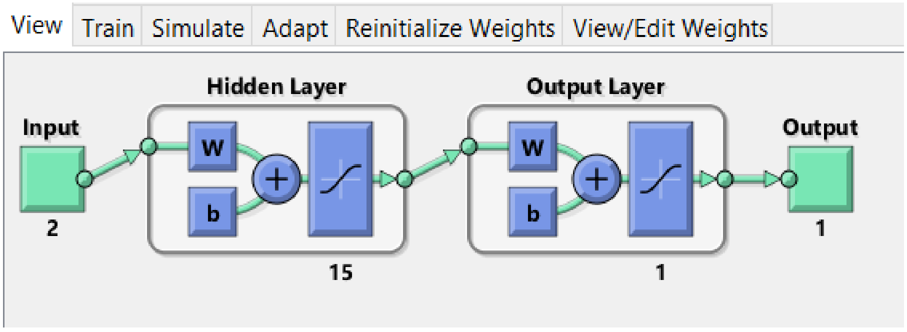

Figure 6. The 2-h (15)-1 neural network studied

3. RESULTS AND DISCUSSION

After having introduced our dataset in the ANN, and after having trained it, the results appearing in the training window are performance and regression plots. The first illustrates performance against the number of iterations. Each of the entire training sets represents an era. At each epoch, the model adjusts the weights automatically to gradually converge towards an optimal set of results. Several periods are often compulsory before the top of the training.

Since the determination of mechanical characteristics is a regression problem, we choose the mean squared error as the objective function, which is denoted mean squared error (MSE) [15]. The mean difference between targets and results is known as the mean squared error, it represents one of the two elements that indicate that the chosen smart model is performing. The second indicator is regression, which is mainly used for validation of the model under study and justifies the link between objectives and results [16]. Our network is made up of two input layers which respectively represent the Young modulus of polypropylene and bio charge, 15 neurons in the hidden, and one output layer which represents the Young modulus of the biocomposite. Table 2 represents the parameters of the chosen network.

Table 2. Parameters of the network chosen

Data division	Training	Performance	Calculations
Random ($dividerand$)	Levenberg – Marquardt ($trainlm$)	Mean squared error (MSE) Regression coefficient (R)	MEX

The activating function of these neurons is $tansig$. This activation function appears to be the best compromise between the different activation functions, sigmoid, and linear [17]. This hyperbolic tangent function is used to activate the network operation, and it is characterized as (1).

$$f(x) = Tanh\ (x) = \left\{\frac{2}{1+e^{-2x}} - 1\right\} \quad (1)$$

The response data from the Mori-Tanaka model is used as input to the model chosen to train it to predict the elastic behaviors of biocomposites. The data was grouped into different sets; 70% for training, 15% for testing, and 15% for validation. The artificial neural network (ANN) was trained through iterative testing and error checking to minimize squared error while maximizing regression values [18]. To avoid overfitting, there are several methods to follow to ensure that the model converges well. We can note the cross-validation [19], the limitation of the number of neurons or the limitation of the training duration [20]. In our case, we used 15 neurons, thus a limited number, and in addition to that, in each training, we kept the model and its characteristics, consequently, this allowed us to avoid overfitting [21]. Figure 7 shows us the training state Data by the feed-forward backpropagation.

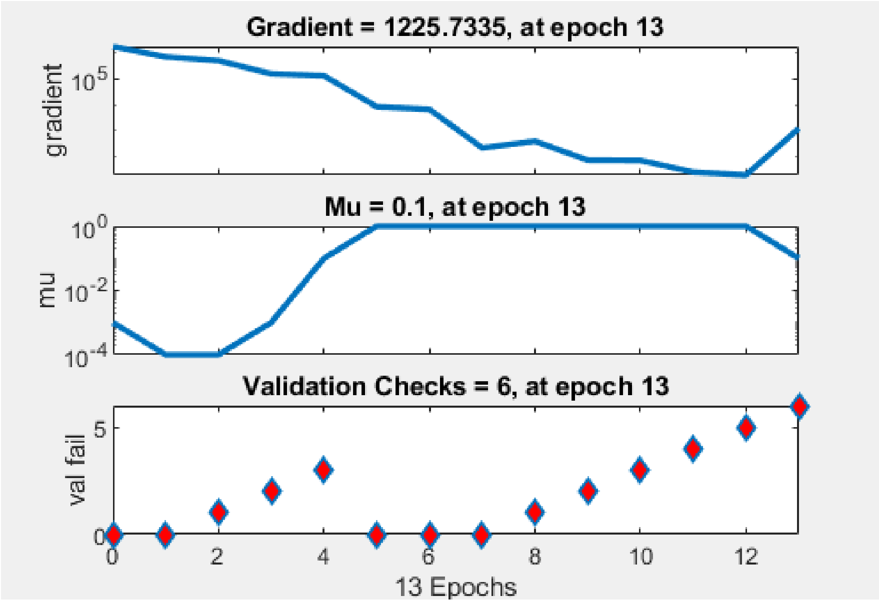

Figure 7. Training state data of neural network

Using 1,000 repeated epochs of training, the mean squared errors (MSE) produced by the feed-forward backpropagation and the regression are as shown respectively in Figures 8 and 9. The three curves, test, training, and validation, follow approximately the same path and gave 15.72 as the best validation performance at 7 epochs. The regression coefficient for polypropylene loaded with 15% bamboo fiber is 0.98, approaching 1, indicating the efficiency and effectiveness of our model [22].

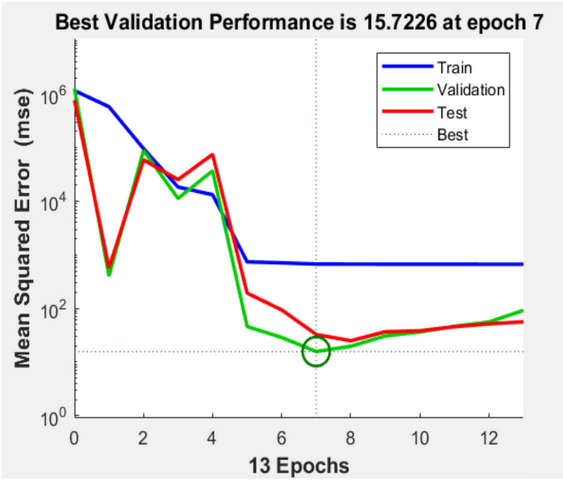

Figure 8. Validation performance

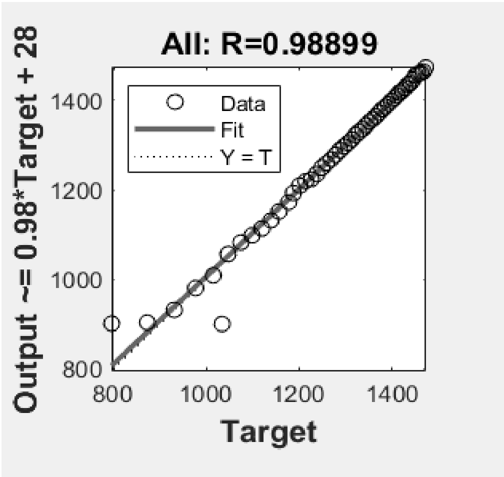

Figure 9. Regression analysis

We followed the regression of the three sets (training, validation, and test) used in the training of the predictive model. Figure 10 shows that their regression coefficients converge towards 1, which further proves that our network is performing well [23]. The correlation between the predicted values from our intelligent model and the target values tends to 1 (0.98), which means that the relationship between these two variables is almost linear [24]. So, our predictive model was able to follow the training and was able to give its output almost identical values similar to those of the Target. Indeed, Figure 11 shows us that the two curves (target and model output respectively) follow the same trajectory and that the difference between the two is almost zero. Hence the accuracy of the response of our predictive model.

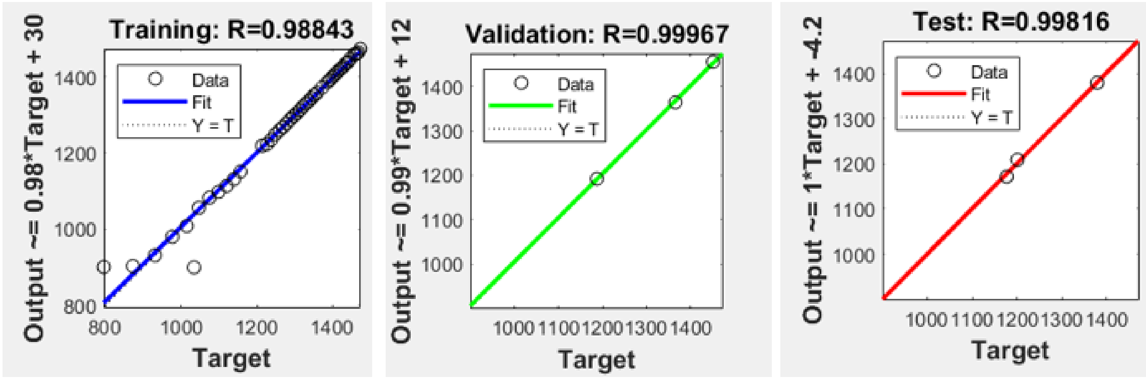

Figure 10. Validation performance of train, validation, and test data

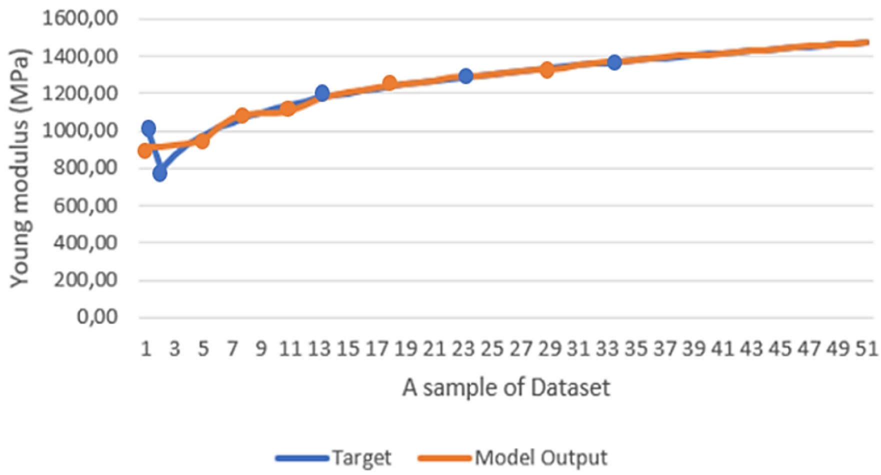

Figure 11. Correlation between dataset values and the predictive values

The different Young's modulus of polypropylene, bamboo fibers, and our biocomposite are represented in Table 3-which contains 85% of PP reinforced by 15% of bamboo fibers, obtained from Mori Tanaka and the intelligent models. From this study, it was proven that the prediction of Young's modulus using artificial intelligence gave an efficient result given that the error is minimal, and this with better validation of performance [25].

Table 3 highlights an increase in the stiffness of 15% bamboo bio-filled PP, marked by an increase in Young's modulus of 550.3 MPa compared to PP without bio-filling. This observation was expected, as the stiffness of the bio-filler is higher than that of the PP matrix. The difference between the numerical values and the results from the artificial intelligence tool is approximately 3.68 e-06, indicating satisfactory accuracy.

Table 3. Different Young modulus studied

Material	PP	Bamboo	Bio composite experience	Bio composite Mori Tanaka	Bio composite ANN
Young Modulus (MPa)	1034	14600	1572.9	1584.3	1584.299

4. CONCLUSION

In this article, we have proposed a feed forward back propagation which represents a form of the Deep neural network method to predict the polypropylene loaded with natural fibers elasticity. Our Feed-forward back-propagation trained by the LM algorithm can efficiently and accurately predict the elasticity of the innovated material by feeding our network by dataset comprising different Young's modulus corresponding to various bio fillers.

This intelligent method is easy to use, and it has broad application perspectives in the modeling of bio-composite materials. It might be noticed that only 85% of polypropylene has been treated as an illustration of this smart method in this article. However, we can extend this method to determine the elastic behavior of biocomposites at different mixing percentages. Furthermore, we can apply this proposed method to calculate and determine other thermomechanical characteristics of biocomposites, we can cite the Poisson ratio, the thermal conduction coefficient, the fatigue resistance, and doing all of this in the shortest amount of time and with the least amount of error.

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