Pentamode Metamaterial Design via Wave Simulation and Machine Learning

MSME Master's Thesis Proposal

The student's name was discarded

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February 1, 2022

1 Introduction

Metamaterials are artificial engineering materials with acoustical, electromagnetic and mechanical properties that have not been found in naturally occurring materials. One of their notable features is that they can mimic the water properties and achieve acoustic invisibility. Therefore, metamaterials have broad application prospects in sound insulation, acoustic cloak, and marine research. Although the corresponding theoretical research has proved the advantages of metamaterials, their applications are still limited by the complexity of the required manufacturing techniques. Engineering software simulation and machine learning technology provide solutions to the above technical problems. The existed lattice structures [1–3] can be improved to meet the requirements of specific appliances, for example, behave as metal water at broad range of frequencies including higher frequencies. This project will verify the manufacturability of pentamode metamaterial structures and optimize the existing models.

2 Literature review

2.1 The development of pentamode metamaterials

The theoretical model of pentamode metamaterial first introduced by Milton and Cherkaev in 1995, is a model of a three-dimensional lattice of a solid structure formed with tetrahedral pentamode unit cells [4]. This structure has a high bulk modulus and low shear modulus. In other words, it can mimic water's properties in underwater acoustic applications. Kadic et al. [5] investigate this pentamode theoretical ideal suggested by Milton and Cherkaev can be approximated manufactured by the by a metamaterial with lithography. They [5] used the finite connection to replace the strictly point-like tips and found the ratio of bulk modulus to shear modulus of the 3D structure can realistically be made as large as about 1000. The feasibility of PM metamaterials acoustic cloaks was theoretically conceived by Milton et al [6] and further improved by Norris [7]. Milton et al [6] studied how the form of the conventional elastodynamic equations changes under curvilinear transformations. Norris [7] showed perfect cloaking can be achieved with finite mass by using anisotropic stiffness. The acoustical parameters like mass density and mechanical stiffness are anisotropic in the cloak. The phase speed and wave velocity of the pseudo-acoustic waves in the cloak are unique for a given transformation mapping. Li et al. [8] verified that the parameters of cell properties are changed independently to satisfy the requirement for the application of acoustic cloak. The acoustic cloak allows the object to be undetected by sound. When sound transmits to the object enveloped by the acoustic cloak, the sound passes through and around the cloak without causing reflection on the surface of the object. In their research [8], the acoustic properties of the lattice structure are adjusted to match with the surrounding medium which is, in this case, water. These characteristics show that pentamode metamaterials have many potential applications and one example is in medical ultrasound imaging. Su et al. [9] designed and fabricated pentamode gradient-index (GRIN) lenses. They [9] tuned the impedance of unit cells to match with water so that the sound is focused with minimal aberration. Huang et al. [10] studied core-shell pentamode metamaterial by using finite element method. Compared with the traditional non-core–shell structure, the new structure effectively improves the ratio of bulk to shear modulus. In other words, it has a broader mechanical response and higher sensitivity. Cai et al. [11] studied four types of anisotropic pentamode metamaterials and investigates how anisotropy affects pentamode metamaterial properties. This research [11] provided a reference to the application of pentamode metamaterials, such as acoustic cloaks and acoustic carpets.

2.2 Applying Deep Learning to metamaterial design

Machine learning [12, 13] is a process that enables artificial intelligence to absorb large amounts of unstructured data (images, texts) and develop a system used to solve a specific problem. Deep learning [12, 13] is a subset of machine learning widely applied to the design of metamaterials. Zhang et al. [14] designed an approach to fast calculate elastic wave properties of digital materials with all orderings and establish a digital structural genome accurately by combining the deep learning with the finite element method. Compared with the traditional method, the new method [14] is more accurate and time-saving to determine the orderings of digital materials. It has a significant meaning for inverse design anisotropy and spatial distribution of materials. Wang et al. [15] developed a meta-modeling framework to generate mechanical constitutive models through deep reinforcement learning. They [15] formulated meta-modeling as a Markov decision process. The policies and state values are estimated by neural networks (NN) such that the computer can self-improve the constitutive model through self-playing. This automated meta-modeling [15] can produce better models that improve prediction accuracy. Wang et al. [16] invented a framework that has a variational autoencoder (VAE) and a regressor for property prediction. The regressor plays a unique role to predict the labels for generated images in the deeper learning network. This method [16] simplifies complex microstructures into a low-dimensional and organized latent space and reduces the high computational cost of the large-scale metamaterial database. In the latent space, simple vector operations are used to tune the microstructures. The VAE can be used to generate microstructures for multiscale metamaterial systems [16]. Shah et al. [17] introduced a semi-analytical method of suppressing acoustic scattering in which a reinforcement learning (RL) agent is used to control the parameters of cylindrical scatterers in water. In this model [17], the RL agent receives a reward that can be maximized to discover designs in low scattering. Nonlocal metasurfaces are used to control sound propagation accurately. But complex coupling hinders further functionality study. Ding et al. [18] proved that preset dataset can be more efficiently learned through deep learning algorithms to explore the potential functionalities of nonlocal metasurfaces. Wiest et al. [1] studied how to improve the feasibility of using additive manufacturing technology for acoustic metamaterials and metasurfaces by multiple methods, including finite element method (FEA), appropriate metamodel for Monte Carlo (MC) simulations. A shallow neural network (NN) architecture, called a multilayer perceptron (MLP) classifier, is a general-purpose nonlinear approximator and has many options for tuning the performance. MLP classifier was used as the metamodel in their research. Their research [1] demonstrated how to use the robust design approach in selecting additive manufacturing fabrication methods and the possibility of fabricating acoustic metasurface with asymmetric absorbing capabilities and well-matched to water.

2.3 Using Generative Adversarial Network for inverse design

Generative adversarial networks (GANs) are neural networks that generate data, such as text and images. Generative modeling is an unsupervised learning task. It allows the model to discover the patterns in input datasets and generate new data which mimic the regularities of the original input data. Goodfellow et al. [19] developed the generative adversarial networks (GAN). The GAN framework contains two network models, generator (G) that captures the data distribution and discriminator (D) that estimates the probability of the output data. Zaghloul et al. [20] built anisotropic radio-frequency (RF) metamaterial unit cells for metasurface (MTS) arrays by employing deep convolutional generative adversarial networks (DC-GANs). The networks have a better understanding of the relationship between the physical structure of meta-atoms and their reflection spectra. The generated array structure [20] has similar features to the given data used in training the model. The traditional ways of designing acoustic metamaterials rely on the expertise of specialists. Marburg et al. [21] invented a new method that uses conditional generative adversarial networks (CGAN) to build a framework. They [21] used the framework to generate unit cells for sound insulation purposes and analyzed the final results by FEM simulation. Raghuvanshi et al. [22] built convolution neural networks for fast acoustic scattering. The traditional method required expensive numerical simulation. However, the new method turned a convex scattering cross-section into a 2D slice. They [22] proved that the full-resolution residual network could generate detailed loudness fields with small root mean square (RMS) loss. Lai et al. [23] presented a method of generating conditional Wasserstein generative adversarial networks (cWGANs) model instead of optimization algorithms to reduce the total scattering cross-section (TSCS) to near zero for a planar configuration of cylinders. The conditional functionality and the coordinate convolution (CoordConv) layer were introduced to the standard WGAN to enable the model to generate design images targeting specified TSCS responses and improve the meta-cluster accuracy and image quality. The R regressor model was trained with the random configuration datasets and used to predict the TCSC from images of either 2- or 4-scatter configurations. They [23] evaluated generated results to demonstrate the capability of the model in producing meta-cluster designs for minimizing the TSCS.

3 Objective

3.1 Objective statement

The objective of this project is to design tetrahedral pentamode cells to construct a 3D lattice structure. The lattice structure will have a high bulk modulus, low shear modulus, and acoustic properties similar to water. The existing models [3] will be modified by altering the property constraints of the unit cell to generate data for the requirements of specific appliances. The dataset will be used to train the neural networks by utilizing multiple machine learning and deep learning algorithms. Finally, the trained neural networks will generate optimized data to improve the structure. The optimized structure will behave as metal water at higher frequencies and has better manufacturability.

3.2 Evaluation metrics

The pentamode cells are designed to mimic the property of water. One of the objectives of this project is to increase the band gap to higher frequencies. The current band gap is between 30-40 kHz. The second objective is to increase the ratio of bulk to shear modulus. The current bulk to shear modulus ratio is about 107.9.

4 Methodology

4.1 Review of the acoustic engineering theories

The project involves multiple engineering theories, from structural analysis to acoustic engineering theories. The transformation acoustic theories [2, 3, 7, 24] will be used as the fundamentals to design the pentamode metamaterial cells for mimicking the acoustic properties of water. These cells cannot be wave propagated in specific frequency ranges called band gaps. The band gaps in periodic elastic structures are caused by the multiple waves scattering at the interfaces between different materials.

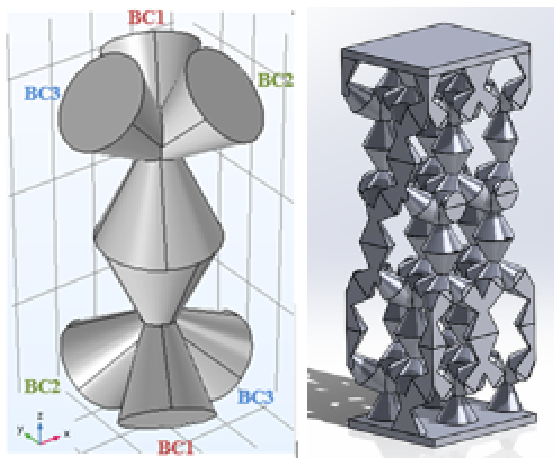
4.2 Model Design and data Collection

The pentamode model studied by Matthew Kelsten et al. [2, 24] from Rutgers University will be used as a reference for my design. The Kelsten's pentamode lattice was manufactured by a 3D Systems ProX DMP 320 Metal printer with the titanium powder, laser form TI Gr23 (A). The sample has dimensions of $98.9 \times 98.7 \times 87.2mm^3$. Two 1.3 mm thick titanium plates were placed to the top and bottom of the sample to prevent water penetration during the underwater testing. In different with Kelsten's model, my model will have the dimensions of $70.7 \times 70.7 \times 97.4mm^3$. The titanium plates placed to the top and bottom of the sample will have the same thickness as Kelsten's model.

Kelsten's design [2, 24] was focused on emulating the acoustic properties of water and exhibiting acoustic anisotropy through the forward methods, such as wave simulation by COMSOL Multiphysics and finite slab simulation. The initial simulations were to study the band structure of propagating bulk modes. The phase speeds in x1- and x2-directions which were less than the sound speed in water were identified as "slow" direction and the phase speed in x3-direction which was higher than the sound speed in water was identified as "fast" direction. Then the simulation of the reflection and transmission effects of the PM, when submerged in water, was taken to anticipate the measurement results. The reflection-transmission analysis shows the in-plane motion (x3-component) is two orders of magnitude greater than the out-of-plane motion (x1 and x2-component). In the full-wave simulation of a slab of PM material, the dispersion effects are proved to be more significant in the slow direction. The results of these simulations agree with each other. The underwater measurements were taken to validate the expected anisotropic acoustic propagation behavior of the 3D printed PM samples. Similar to Kelsten's design, my model will be simulated through COMSOL multiphysics to calculate the wave speed in x-, y- and z-directions on the dispersion curve. Kelsten et al. [2, 24] studied the key PM features and proved the 3D PM materials can be created using additive manufacturing.

The pentamode model studied by Anam Abbas [3] from San Jose State University will also be used as a reference for my design. Abbas studied the related model not only by using wave simulation as the forward method but also through deep learning techniques as the inverse design method, including Python Tensor Flow and Keras API. Wasserstein generative adversarial network and gradient penalty (WGAN-GP), a conditional generative adversarial network, was used in the inverse design as an alternative to clipping weight for improving stability. Abbas [3] proved that the titanium lattice structure can transmit waves through it with minimum back scattering and the lattice structure behaves as metal water between the frequencies of 20 to 30kHz. My design will further increase the band gap range so the cell could behave as metal water at higher frequencies.

The 3D model of the unit cell presented in Fig.1a is used for the preliminary work. The unit cell is a face-centered cubic diamond-shaped lattice structure made up of cone linkages. The unit cells are constructed in SOLIDWORKS and assembled to a lattice structure (Fig.1b) before importing to COMSOL. The displacements, stresses, strains, eigenfrequency, eigenmodes, and resultant frequencies are calculated, and the interface study are conducted on the lattice structure. The pressure acoustic frequency domain interface study is set up by coupling the acoustic-solid interaction multiphysics with the frequency domain. It computes the pressure variations of acoustic waves' propagation in fluids at quiescent background conditions. Finally, the parameters of model are recorded in the excel file and split randomly into a training and testing set and loaded to the networks as a CSV file.



(a) Unit cell structure (b) Lattice structure

Figure 1: PM structure adapted from [3, 24].

For the lattice structure, the effective density is calculated by the following equation[3].

$$\rho_{eff} = \frac{\rho_s V_s}{V_{cell}}$$

Here ρ_s is the density of solid Titanium, V_s and V_{cell} are the volume of the PM structure and the volume of the unit cell, respectively.

The bulk modulus B and shear modulus G are calculated by the following equations[3].

$$B = c_B^2 \rho_{eff} - \frac{4G}{3}$$

$$G = c_G^2 \rho_{eff}$$

Here c_B is compression wave velocity and c_G is shear wave velocity can be obtained by dispersion curves.

4.3 The training process of the neural networks

4.3.1 Training with deep neural networks

The data and images collected through previous wave simulation will be used to train the neural network. The neural network consists of an input layer, two hidden layers with 64 and

32 neurons, and an output layer. Four input parameters are the height of the base cone, the ratio of base cone radius vs. small cones base radius, the ratio of bulk to shear modulus, and the impedance of cells structure. The four output values are the ratio of base radius to the tip radius, the ratio of height to the base radius, the cone connecting angle, and the density of cells structure.

The training process contains multiple deep learning algorithms, including mean absolute error (MAE) loss function for estimating the difference between actual and predicted output values, mean squared error (MSE) loss function for minimizing the variance (increase accuracy) in the training data, and rectified linear unit (Relu) activation for increasing computational efficiency by adjusting the weight of the input values to minimize the error function. To evaluate the network, the dataset will be split into a training set and a validation set by using the K-fold cross-validation method. It minimizes the MSE values by splitting the data into k partitions where k=4 and trains each one with k-1 partitions. The validation score is the average of the k validation scores obtained.

4.3.2 Training with generative adversarial networks

In the inverse design process, generative adversarial networks (GAN) will be used to take data augmentation. GAN comprises two convolutional networks, discriminator, and generator. The discriminator maximizes the probability of distinguishing if the image comes from the real or generated dataset. The generator minimizes the difference between the real and generated images. Wasserstein GAN will further improve the stability of the training process. The loss function for GAN is calculated by the following equation[3].

$$\underset{G}{min}\underset{D}{max}E_{p_r}[log(D(x))] + E_{p_g}[log(1 - D(\bar{x}))]$$

Here E is the expectation, P_r and P_g are the probability distribution of real and generated data. The real data is fed to the discriminator D(x) and the generator is fed with random noise in latent space $D(\bar{x})$.

For Wasserstein GAN, the total loss for the model is the sum of the critic and the gradient penalty loss which calculated by the following equation[3].

$$L = E_{p_g}[D(\bar{x})] - E_{p_r}[D(x))] + \lambda E_{p_z}[(||\nabla_x D(\widehat{x})||_2 - 1)^2]$$

Here P_z is the probability of random samples from $D(\bar{x})$, which consists of samples from real and generated data.

4.3.3 Training with variational autoencoder

I will use variational autoencoder (VAE) [25] as an alternative method to avoid over-fitting and ensure the latent space will have good properties to generate new data. VAE is a probabilistic generative model that uses Bayesian inference to approximate the distribution of data. The true distribution of input images $P_\theta(x)$ is calculated by the following equation[25].

$$P_\theta(x) = \int P_\theta(x|z)P(z)dz = \int P_\theta(z|x)P(x)dz$$

Here $P(z)$ is the predefined distribution, x is the input data, z is the latent variable drawn from $P(z)$, θ is the model parameter.

4.4 Preliminary Work

The object of the preliminary work is to utilize COMSOL simulation and machine learning algorithms to evaluate multiple methods for predicting the band gap of the unit cell. The unit cell is constructed in SOLIDWORKS and then imported to COMSOL where the boundary conditions and material properties such as Young's modulus, density, and Poisson's ratio are set for the model. The four parameters were chosen as the input values of the neural networks and can be modified easily within COMSOL. The constraints are set for these parameters to limit the gap between the cells for several reasons which include the feasibility of manufacturing, the limitation of structure density, and for the impedance to match that of water. The parameter chose to modify are the height of the cone, the ratio of base cone radius vs. small cone base radius, the ratio of height vs. base cone radius, the cone connecting angle. The parametric sweep study was then taken to plot the dispersion curve. The values of the upper and lower boundaries of the band gap were chosen as the output values of the neural networks. The four input and two output values are recorded in the excel file for training the neural networks. The total number of the datasets is 240.

The training process contains the following scenarios: one with K-fold cross-validation, one with traditional training validation, one without a validation dataset, and four models of bagging, random forest tree, boosting, and stacking. The predicted and real values of each scenario are compared to determine the accuracy of each method for predicting the band gap range.

In the first scenario, the k-fold cross-validation method is used to split the data into four partitions. Fig.2a demonstrates a dramatic drop for MAE values after about 25 epochs. Fig.2b shows the comparison between the real and predicted values. The comparison shows the high accuracy for the k-fold cross-validation method. The real and predicted values are very close.

In the second scenario, the traditional training validation method is used to split the data into four partitions. The test data was split into training and validation data sets with a ratio of 3:1. Fig. 3a demonstrates a drop in loss values after about 150 epochs. Fig.3b shows the comparison between the real and predicted values. Compared with the k-fold cross-validation method, the drop for loss values is slower and errors between the real and predicted values are larger.

In the third scenario, the networks don't have validation datasets. Fig.4a shows the comparison between the real and predicted values. Compared with the k-fold cross-validation method, the errors between the real and predicted values are larger. Then the learning rate of Adam is changed to 0.01 for getting a better result. Fig.4b shows the comparison between the real and predicted values. The errors are as small as the k-fold cross-validation method. So, the conclusion is that methods of the k-fold cross-validation and the setting of the learning rate of Adam to 0.01 are both effective in predicting the bandgap range.

The neural networks are trained in addition to four models including, bagging regressor, random forest tree, boosting and stacking. Fig.5a shows the comparison between the target and predicted data for the bagging regressor model. The errors between them are the largest among the four models and especially large when predicting the maximum values. Fig.5b shows the comparison results for the boost model. The predicted results are more accurate than the bagging regressor model. But errors are still obvious near the critical points. Fig.5c and Fig.5d show the comparison results for the random forest tree and stacking model. For these two models, although some errors still exist, their predicted results are the most accurate among the four models.

Through the preliminary work, the unit cell is fully studied as the preparation for the further study of the assembled lattice structure. Multiple machine learning algorithms are used to train the neural networks as fundamental for the utilization of more complex convolutional neural networks (CNN) and generative adversarial networks (GAN).

NOTE: The preliminary data presented in Figures 2, 3, 4, and 5 was discarded in the Sample Proposal as the data was not published yet.

4.5 Risks and Contingencies

The risk during this project is the inverse design of the neural network. An ideal neural network requires a large quantity of data for training purposes. The data generated by the lattice study may not be enough. So, choosing efficient algorithms will be crucial for the build of the neural network.

4.6 Resource

Resources	Time needed by	Cost	Source
SOLIDWORKS license for 3D modeling and 2D drawings	January 2022 - December 2022		SJSU student license
COMSOL license for 3D modeling and 2D drawings	January 2022 - December 2022		SJSU student license SJSU Virtual Desktop Infrastructure (VDI) access
Titanium powder for building a lattice structure	October 2022 - December 2022	$ 300	Apply the funds through Davidson Scholarship
HPC clusters, Docker systems with new GPU computer	2022		Work with Professor Amirkulova

Figure 2: The resource for the project

4.7 Proposed research/work

The current lattice structures in Anam Abbas [3]'s and Matthew Kelsten [2, 24] 's research have been fully studied firstly as the reference in building the new 3D lattice structure. The new structure will be constructed based on the existing unit cell model using Livelink for SOLIDWORKS to set up COMSOL simulation. The structure will be taken full-wave simulation to ensure it matches water's acoustic impedance and achieves high bulk modulus and low shear modulus. The properties of the structure will be altered during the simulation and collected to set up datasets for training the deep neural networks. During the training of the neural networks, multiple algorithms proved to be effective in Abbas's research [3] will be applied. These algorithms include K-fold cross-validation, mean squared error (MSE) loss function, mean absolute error (MAE) loss function, and rectified linear unit (Relu) activation. The variational autoencoder (VAE) [25] will be used as an alternative method to avoid over-fitting and ensure the latent space will have good properties to generate new data. The next step is to set up conditional Wasserstein generative adversarial networks with gradient penalty (cWGAN-GP) to generate images and labels. A convolutional neural network (CNN) will be used as an auxiliary regressor to predict all design parameters for the cell images. The method used in Peter Lai's research [23] about reducing the total scattering cross-section (TSCS) for a planar configuration of cylinders by cWGAN model will be used as the reference. The conditional functionality and the coordinate convolution (CoordConv) layer will be introduced to the standard WGAN for generating images. Finally, the output results of properties of the structure will be used to construct a lattice structure through COMSOL Multiphysics for testing.

5 Deliverables and Task

Deliverable 1. A 3D model built by SOLIDWORKS and COMSOL for full-wave simulation.
  Task 1.1 Build pentamode unit cells and take the parametric study
  Task 1.2 Assemble the cells to build a lattice structure
  Task 1.3 Full-wave simulation of the model
Deliverable 2. The lattice structure optimized through the deep learning process.
  Task 2.1 Generate dataset for training networks
  Task 2.2 Take forward study of the model
  Task 2.3 Inverse study via generative adversarial network (GAN)
Deliverable 3. Submit abstract and deliver the progress project and the oral presentation in May at ASA Spring 2022 meeting in Denvor, CO and present it at IMECE 2022.
Deliverable 4. Prepare manuscripts for a journal publication and/or a conference paper.

6 Timeline

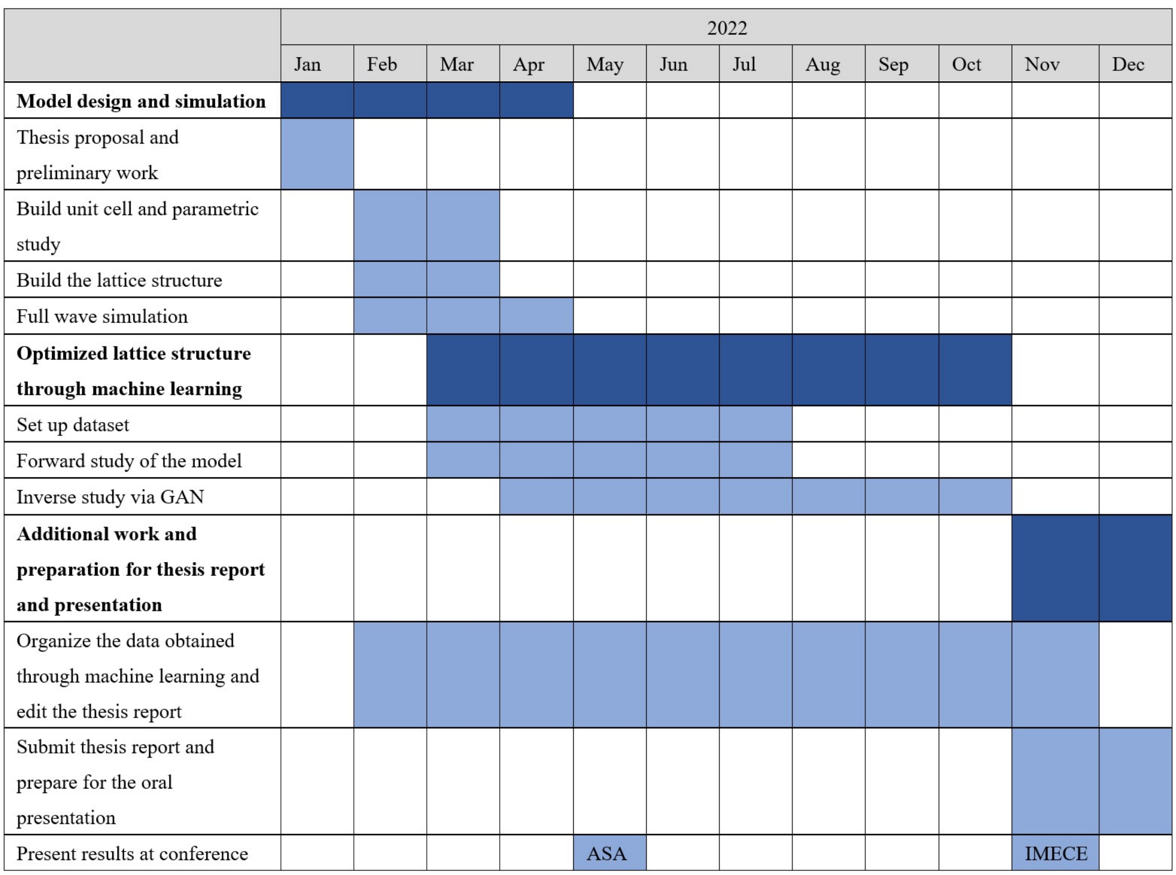


Figure 3: The timeline for the project

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