Generative Artificial Intelligence for Metamaterial Design

A Major Qualifying Project

submitted to the Faculty of

WORCESTER POLYTECHNIC INSTITUTE

in partial fulfillment of the requirements for the

degree of Bachelor of Science

by

Priya Natarajan

Date:

August 2023

Report Submitted to:

Professor Lin Cheng
Worcester Polytechnic Institute

Abstract

Metamaterials created through artificial intelligence (AI) models are a new way to engineer materials with a wide range of properties. Variational autoencoder (VAE) is an AI model that allows engineers to quickly design materials with specific properties from the latent space. The motivation for this paper is learning how to use AI as a tool for future architectural engineers. Creating new meta materials with complex geometry allows architectural engineers to design sustainable buildings and cities with strong materials. The methods of this paper describe the research that has been done, including running codes for different AI models and utilizing VAE model for generating materials. The results look at the output generated by the code and its application towards various fields including architectural engineering is discussed. The discussions observe the importance of using AI as a tool for faster decision making. The conclusions discuss the future of AI.

Introduction

Metamaterials are artificial materials that have specific material properties and have been broadly applied in various fields, as shown in Figure 1 [1]. Metamaterials can be represented by using a regular mesh, in which each voxel in the mesh represents a building block for the construction of microstructures. By developing different combinations of voxels within the design domain, it is possible to achieve unprecedented properties that cannot be achieved by using single solid materials. Although metamaterials exhibit excellent performance in various applications, it is challenging to design metamaterials. This is because the computational cost of searching for the desirable microstructures from infinite candidates is too expensive [2].To overcome aforementioned challenges, AI, especially generative AI models, is introduced to design metamaterials with specific properties. AI models use powerful computers to mimic the neural connectivity of the human brain and allow universal approximation of complex interpolation functions [3]. This can help to design these complex multi-scale metamaterial in a low dimensional latent space [4].

I am motivated to learn about metamaterials because they can be applied towards a wide variety of engineering fields, most notably architectural engineering [5]. Metamaterials are modeled after metals and plastics, which are common building materials for architectural engineers. Metamaterials are important for architectural engineers because they provide multifunctional performance by fine tuning the materials' microstructure. In this project, I used variational autoencoders (VAEs) to generate materials. VAEs describe in a detailed manner the probability of several different observations happening in a latent space. Figure 2 describes the process of the VAE for metamaterials development. The input variable goes into the encoder and comes out of the decoder. The encoder is the process that produces new features based on latent space. The decoder does the reverse of the encoder, going from the samplings to the microstructure design.

The result includes a latent space describing the probability of this variation and the reconstructed metamaterial [6]. The encoder and decoder work together while automatically performing the calculations to determine the values faster than calculations done manually [7]. Conditional variational autoencoders (cVAEs) are the same basis but have an additional condition in between the input and output, allowing for a more precise observation [8]. I also did research on stable diffusion, which is a more advanced model that allows the input to be a text prompt, and the output be an image generated based off the prompt.

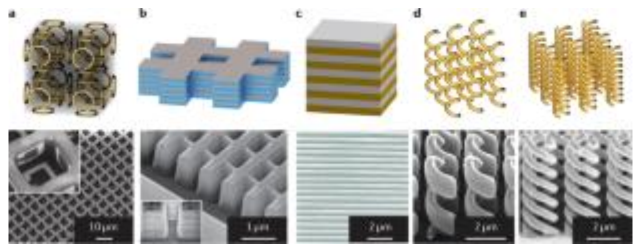

Figure 1: This is a gallery of 3D metamaterials [9].

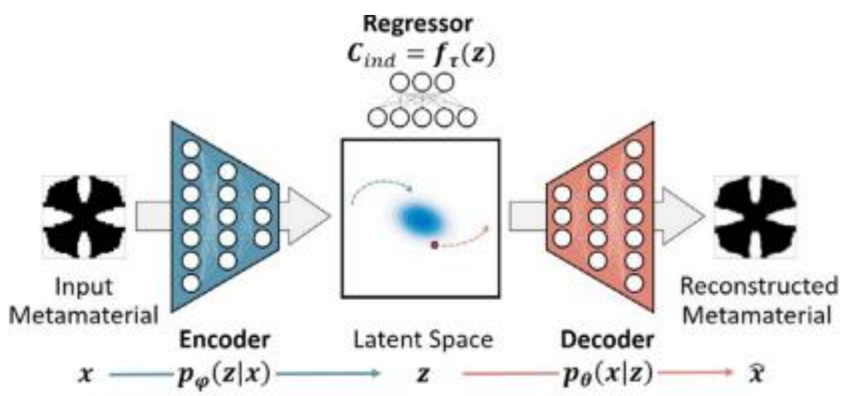

Figure 2: Schematic illustration of VAE model for metal materials development. [10]

State of the Art

Recently, more people have conducted research on applying deep neural networks and deep machine learning for structure and material designs. This includes both predictive models and generative models [11]. Predictive models predict a given design's performance and aim to lower the computational cost associated with an AI model [12]. Deep generative models learn the underlying structure of a given dataset to generate innovative designs in a low latent space. Examples of deep generative models are Generative Adversarial Networks (GAN) [13] and Variational Autoencoders (VAEs) [14]. Deep generative models have been applied towards reconstructing micro materials [15].

In this project, I chose to use VAEs to design metamaterials. By using datasets provided by Professor Cheng. VAEs can learn the structure and generate new structures of materials. The VAEs can develop new geometries and properties of metamaterials that are not provided in the database. Extensive research helps understand the process of AI through VAEs. Understanding Python and coding is an essential part of AI development. VAEs use Stochastic Gradient Bayes Framework and Gaussian Latent Variables in their computations to estimate the likelihoods of an outcome. The goal is to create robust structured predictions. The following equation describes this framework:

$$-KL\left(q\varphi\big(z|(x)|\big|\big(p\theta(z)\big)\ +\ E_{q\varphi}[\log p\,\theta(x|[(z)]|)]\big|\big)\right)$$

This equation describes the lower bound calculations of the input x and z in the latent space. X is the data the model is trained on. Z is hidden data of X in latent space. $q\varphi(z|x)$ represents the recognition distribution. $p\theta(x|z)$ represents the approximate true postier. AI repeats these calculations for several inputs, allowing for faster results [16].

Data Collection and Preparation

The data used to train the VAEs in this project is provided by Professor Cheng. Additional data used is from the CelebA [17] and MINST dataset [18] to learn the VAEs. Professor Cheng's dataset consists of metamaterials with randomly sampled fibers in a squared matrix material. The properties that the VAEs use to train the materials include various mechanical properties, such as Young's modulus and Poisson's ratio. The loss function computes the mean square error between the input image and the reconstructed image. The lower the number, the better the reconstruction of the original design from the latent space.

The following images are composite materials consisting of two base materials from the database. One is the matrix materials, represented by the pink color, while the other is the inclusion materials, represented by black color. The differences of the composite materials include the size of the circular cylinder and the locations of the cylinder (inclusion materials).

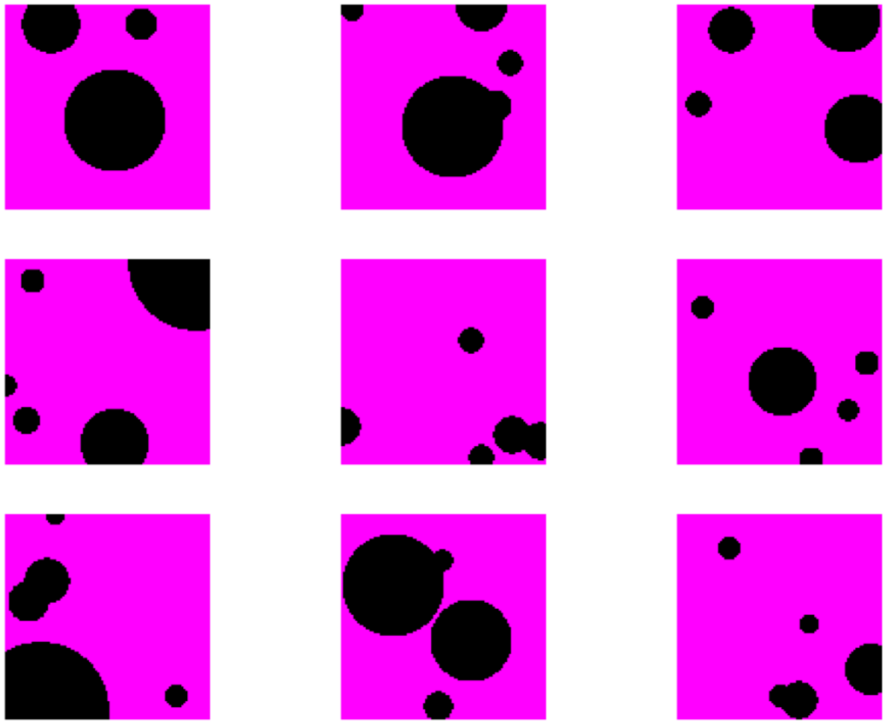

Figure 3: Sample images from Professor Cheng's dataset.

Results

The architecture of the VAEs model contains encoder, decoder, and latent space. The encoder is a neural network that converts data into the latent space. The decoder reconstructs the data given in the hidden distribution. The latent space is a representation of compressed data that allows for easy random sampling and interpolation. The input of the code is images as shown in Fig. 3 while the output of the model is the same materials. The aim of the VAEs model is to replicate the input metamaterials and learn the latent space of the materials properties. Once the model is well trained, new materials can be generated by the decoder of the VAEs model from latent space. The loss function in the code estimates the differences between the predicted and ground truth microstructures. The optimizer of the code aims to optimize the weights and biases of the VAEs model and minimize the loss function.

VAEs can take an image that represents a material with a certain density or other property and generate new images by the learned latent space. The VAEs code used to create new composite materials and generates images through Python Matplotlib library. The loss function, as shown in Figure 4, shows the loss against the epoch.

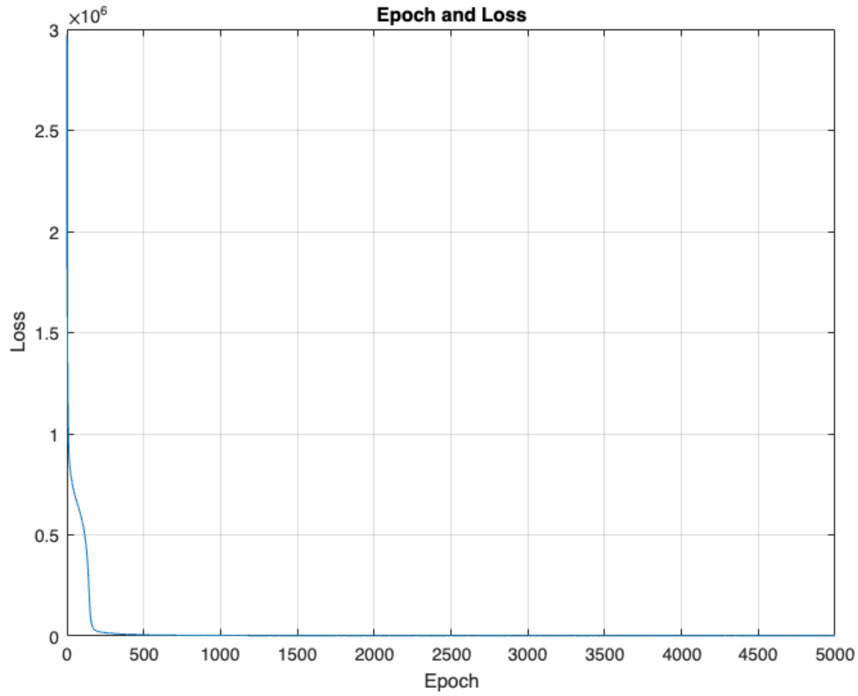

Figure 4: Epoch loss over time for the VAE model used in this project. The goal is to minimize the loss to optimize the model.

```python
device = 'cuda' if torch.cuda.is_available() else 'cpu'

2 usages
class VAE(nn.Module):
    def __init__(self, image_channels, image_size, hidden_size, latent_size):
        super(VAE, self).__init__()

        self.image_channels = image_channels
        self.image_size = image_size

        # Encoder layers
        self.encoder = nn.Sequential(
            nn.Conv2d(image_channels, 32, kernel_size=4, stride=2, padding=1),
            nn.ReLU(),
            nn.Conv2d(32, 64, kernel_size=4, stride=2, padding=1),
            nn.ReLU(),
            nn.Flatten()
        )

        # Latent layers
        self.fc_mean = nn.Linear(64 * (image_size // 4) ** 2, latent_size)
        self.fc_logvar = nn.Linear(64 * (image_size // 4) ** 2, latent_size)

        # Decoder layers
        self.decoder = nn.Sequential(
            nn.Linear(latent_size, 64 * (image_size // 4) ** 2),
            nn.ReLU(),
            nn.Unflatten(1, (64, image_size // 4, image_size // 4)),
            nn.ConvTranspose2d(64, 32, kernel_size=4, stride=2, padding=1),
            nn.ReLU(),
            nn.ConvTranspose2d(32, image_channels, kernel_size=6, stride=2, padding=1),
            nn.Sigmoid()
        )

    1 usage
    def encode(self, x):
        hidden = self.encoder(x)
        mean = self.fc_mean(hidden)
        logvar = self.fc_logvar(hidden)
        return mean, logvar
```

Figure 5: Screenshot showing architecture of the VAEs model.

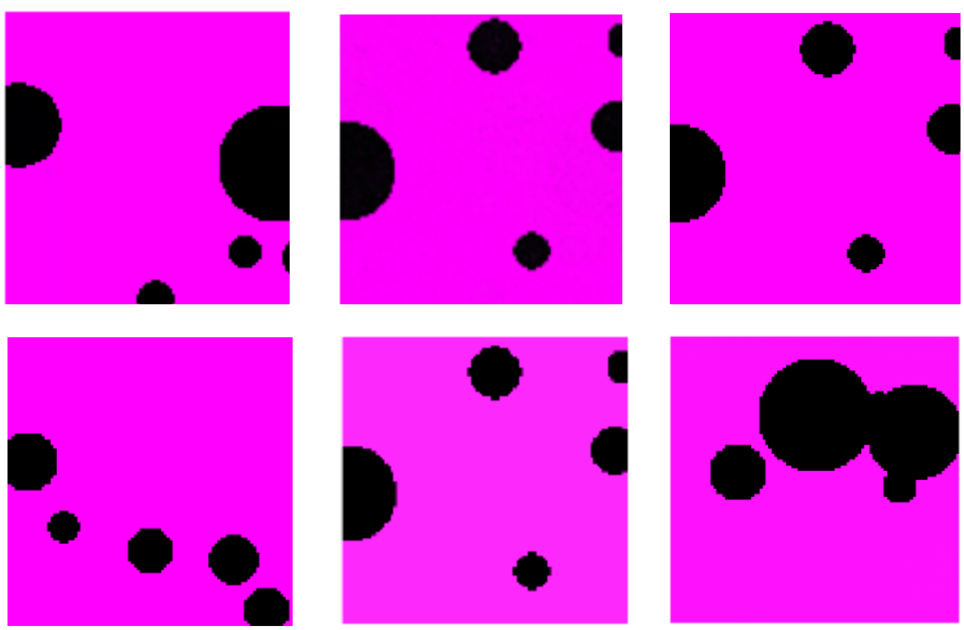

Figure 6: Clear results from the VAEs model.

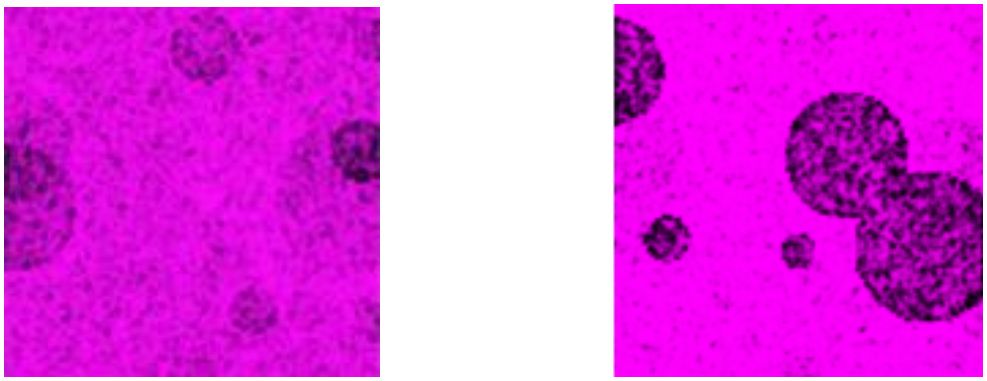

Figure 7: Blurry results from the VAEs model.

Figure 5 shows the architecture of the code and how the data was loaded into the code. The data loader makes the data specific batch size. After that, it passes through the dataset in a random order. Then, it goes through the encoder and decoder. Finally, a reconstructed image is generated.

The VAEs model takes an image of the material and transforms and restructures it into a new image. Figure 6 consists of images generated by the VAE model trained on Professor Cheng's dataset. The results are good because of the clarity of the image and the material.

Figure 7 contains results that are not good because the image is very blurry, and it is hard to distinguish the varying geometries from each other in the image. The limitation of the VAEs is that not all results will be clear images. To fix this problem, the VAEs model needs more training to produce clearer results and physical constraints should be added in the future.

Stable Diffusion AI Model in WPI's Architectural Engineering Program

During WPI's Architectural Design Studio III course (AREN 3002), AI was introduced to students during the conceptual design phase of the studio project. Color.io is a stable diffusion AI model that is available online for free and generates an image based off a prompt. The project was to design a museum of emotions. The following images are from my project and were used as inspiration and a model to design the museum's exterior and the spaces within it.

Figure 8: The color.io stable diffusion method allows for both detailed and broader statements. The type of drawing, shape, and materials are inputted. Within a few minutes, through the power of AI, several images were generated. Specific prompts are used to meet the guidelines and vision of the architectural engineer, but the variation in the images generated goes beyond what the engineer could have produced.

Figure 9: With the same prompt, quite different spaces are reflected in the images generated by color.io.

Figure 10: This image uses AI to produce the foundational drawings. The drawings are all generated by AI.

AI can also be used to create new materials for architecture through VAEs. Materials with different properties, such as Poisson's ratio, are integral for following all appropriate building codes. For example, most commercial buildings use type II-B construction. According to this construction, the minimum fire-resistant rating for building materials is 2 hours for exterior, and 1 hour for interior [20]. Exterior walls that extend below the elevation are required to be constructed with flood-resistant materials [21]. Earthquake and seismic load resistant materials are also important to consider when constructing buildings, as many parts of the country have experienced earthquakes [22].

Also, soundproof materials are increasing in popularity and necessity. Many people live in townhouses, apartments, or close to their neighbors. Everyday tasks can be quite loud for neighbors and take away privacy without soundproof materials. A Vitamix blender's noise is around 90 decibels [23]. To not disturb neighbors, the materials should be soundproof rated to handle prominent levels of decibels.

There are several factors to consider when deciding what materials to use, but the cost is what limits clients and engineers. AI can produce new ways to combine and create new materials that have multiple properties with the same material.

Discussion

VAEs use mathematical equations to encode, decode, and estimate the reconstruction loss. This valuable AI process can be used to decide on the most efficient and effective solution with the lowest reconstruction loss.

The computational cost of running AI models is very high for normal CPU computers. For example, my computer at home is a regular CPU computer, and it took 9 and a half hours to run a stable diffusion code. Using high performance GPU computers specifically designed for AI, I took the same code, and it ran in seconds.

AI allows architectural engineers to broaden their perspectives by generating images of new metamaterials. These artificial materials are completely generated by AI. The AI models are trained on a dataset of different material properties. The models create an abstract space of concepts, such as low Poisson's ratio or high stiffness, and form a conceptual space. In this space, the encoder and decoder store the latent vectors, and the result will be a metamaterial that follows the specific concepts contained in the conceptual space [24].

AI is also being used to create new materials, and will help architectural engineers design energy efficient, safe, and sound buildings for future generations.

Conclusions

Deep learning models allow engineers to model new metamaterials with different geometries and properties. In this project, I used VAEs to model these complex metamaterials in a low dimensional latent space. I also conducted research on stable diffusion, which builds upon this architecture and allows people to input prompts and receive an image as the output. For future work, we should continue to train VAEs models to produce clear images while limiting the epoch loss. Continuing to advance AI models of metamaterials will allow society to engineer a better future, because AI is the future.

Acknowledgements

I would like to acknowledge and thank Professor Cheng for his time spent with me on this project. I would also like to thank WPI's Academic and Research Computing Department for providing me with access to a Turing account. I would like to acknowledge and thank Professor Cheng's PhD student Alex Galvan for creating an account on the remote desktop through NoMachine for me and helping me with coding.

References

[1] Sohn, K., Yan, X., Lee, H., (2015). *Learning structured output representation using deep learning.* https://papers.nips.cc/paper/2015/file/8d55a249e6baa5c06772297520da2051-Paper.pdf

[2] Science Direct (n.d.), *Metamaterials – an overview.* https://www.sciencedirect.com/topics/materials-science/metamaterials

[3] IBM, (no date), *What is Artificial Intelligence (AI)?*. https://www.ibm.com/topics/artificial-intelligence

[4] Liwei Wang, Yu-Chin Chan, Faez Ahmed, Zhao Liu, Ping Zhu, Wei Chen, (2023). *Deep generative modeling for mechanistic-based learning and design of metamaterial systems, Computer Methods in Applied Mechanics and Engineering.* https://doi.org/10.1016/j.cma.2020.113377 (https://www.sciencedirect.com/science/article/pii/S0045782520305624)

[5] Chenxi Lu, Mengting Hsieh, Zhifeng Huang, Chi Zhang, Yaojun Lin, Qiang Shen, Fei Chen, Lianmeng Zhang, Architectural Design and Additive Manufacturing of Mechanical Metamaterials

https://doi.org/10.1016/j.eng.2021.12.023.(https://www.sciencedirect.com/science/article/pii/S2095809922003654)

[6], Rocca, J., (2021, December 11), *Understanding Variational Autoencoders (VAES) - towards data science.* https://towardsdatascience.com/understanding-variational-autoencoders-vaes-f70510919f73

[7], Rocca, J., (2021, December 11), *Understanding Variational Autoencoders (VAES) - towards data science.* https://towardsdatascience.com/understanding-variational-autoencoders-vaes-f70510919f73

[8] GeeksforGeeks, (2022), *Variational Auto Encoders*. *GeeksforGeeks*. https://www.geeksforgeeks.org/variational-autoencoders/

[9] Kadic, M., Milton, G.W., van Hecke, M. *et al.* 3D metamaterials. *Nat Rev Phys* **1**, 198–210 (2019). https://doi.org/10.1038/s42254-018-0018-y

[10] Sohn, K., Yan, X., Lee, H., (2015). *Learning structured output representation using deep*

learning. https://papers.nips.cc/paper/2015/file/8d55a249e6baa5c06772297520da2051-Paper.pdf

[11] Sohn, K., Yan, X., Lee, H., (2015). *Learning structured output representation using deep learning.* https://papers.nips.cc/paper/2015/file/8d55a249e6baa5c06772297520da2051-Paper.pdf

[12] Sohn, K., Yan, X., Lee, H., (2015). *Learning structured output representation using deep learning.* https://papers.nips.cc/paper/2015/file/8d55a249e6baa5c06772297520da2051-Paper.pdf

[13] Yunwei Mao et al. "Designing complex architectured materials with generative adversarial networks," (2020). https://www.science.org/doi/10.1126/sciadv.aaz4169

[14] Liwei Wang, Yu-Chin Chan, Faez Ahmed, Zhao Liu, Ping Zhu, Wei Chen, (2023). *Deep generative modeling for mechanistic-based learning and design of metamaterial systems, Computer Methods in Applied Mechanics and Engineering.*

[15] Sohn, K., Yan, X., Lee, H., (2015). *Learning structured output representation using deep learning.* https://papers.nips.cc/paper/2015/file/8d55a249e6baa5c06772297520da2051-Paper.pdf

[16] Sohn, K., Yan, X., Lee, H., (2015). *Learning structured output representation using deep learning.* https://papers.nips.cc/paper/2015/file/8d55a249e6baa5c06772297520da2051-Paper.pdf

[17] CelebA Dataset (2021). *Large-scale celebfaces attributes (celeba) dataset*. http://mmlab.ie.cuhk.edu.hk/projects/CelebA.html

[18] MNIST handwritten digit database, *The mnist database*. Yann LeCun, Corinna Cortes and Chris Burges. (n.d.). http://yann.lecun.com/exdb/mnist/

[19] Wikimedia Foundation. (2023, August 4). *Variational Autoencoder*. Wikipedia. https://en.wikipedia.org/wiki/Variational_autoencoder

[20] IBC, (2021), *International Building Code.* https://codes.iccsafe.org/content/IBC2021P2

[21] FEMA, (no date), Contract provisions guide - fema.gov. https://www.fema.gov/sites/default/files/documents/fema_contract-provisions-guide_6-14-2021.pdf

[22] SDPWS. (2015). *American Wood Council*. https://awc.org/publications/2015-sdpws/

[23] Press to Cook, (2023), *Vitamix vs. noise: What you need to know before you buy*. https://www.presstocook.com/vitamix-vs-

noise/#:~:text=In%20the%20end%2C%20Vitamix%20blenders,between%2085%20and%2089%20dB.

[24] Liwei Wang, Yu-Chin Chan, Faez Ahmed, Zhao Liu, Ping Zhu, Wei Chen, (2023). *Deep generative modeling for mechanistic-based learning and design of metamaterial systems, Computer Methods in Applied Mechanics and Engineering.*
https://doi.org/10.1016/j.cma.2020.113377
(https://www.sciencedirect.com/science/article/pii/S0045782520305624)