

Intelligent optimization design of new thermal insulation composite materials based on fused deposition molding printing technology

My research field is about the coupling design of materials or structures, in which we hope to use deep learning, Bayesian learning or other data mining techniques to find the complex relationships between variables of engineering problems, and then use some intelligent algorithms, like genetic algorithm, to find the optimal solution. This process may also be called inverse design, and we collectively refer to the technologies used above as artificial intelligence technologies.

This report includes the following three parts. **Background and motivation** will briefly introduce the motivation for applying artificial intelligence technologies to the field of additive manufacturing, and the background of the project I am doing. **Research contents and methodology** will discuss the construction of the training database and the possible deep learning algorithms we want to use. Finally, the **Discussion** part will discuss the significance of deep learning on my field.

Background and Motivation:

Additive manufacturing is growing rapidly for its ability to fabricate parts with complex features. However, the process of additive manufacturing is an extremely complex system involving multi-factor, multi-level, and cross-scale coupling involving materials, structures, multiple physical and chemical fields[1], which makes it easy to produce defects such as pores, non-fusion, cracks, etc. Olson[2] introduced system engineering ideas into the process of material design and structure control and proposed the concept of multi-scale structural design using the integration of multi-level structure simulation technologies. But for the simulation of complex problems, due to the limited knowledge, researchers have to make some assumptions that cause some inevitable modeling errors, and the inheritance of these errors from the multi-level simulation will make it hard to obtain a reliable prediction of the final overall properties[3]. Simultaneously, simulation technology also faces the limitation of computational cost. For example, Yan et al. [4] needed 140 hours of calculation time to simulate a melting process of only 4ms.

For the above problems, the emerging artificial intelligence technology represented by deep learning and data mining provides a new research paradigm for scientific and engineering research [5]. Kalidindi et al [6] demonstrate a novel data science workflow to extract process-structure-properties linkages. Yeong et al[7] reviewed the applications of machine learning in additive manufacturing. The multiscale and hierarchical simulation can be used to offer knowledge and data for the construction of deep learning models, and the probability-based research framework can take the simulation errors into consideration. Therefore, based on artificial intelligence technology, developing intelligent additive manufacturing technology with controllable structure and properties is

one of the most important research directions of additive manufacturing in the future. [1].

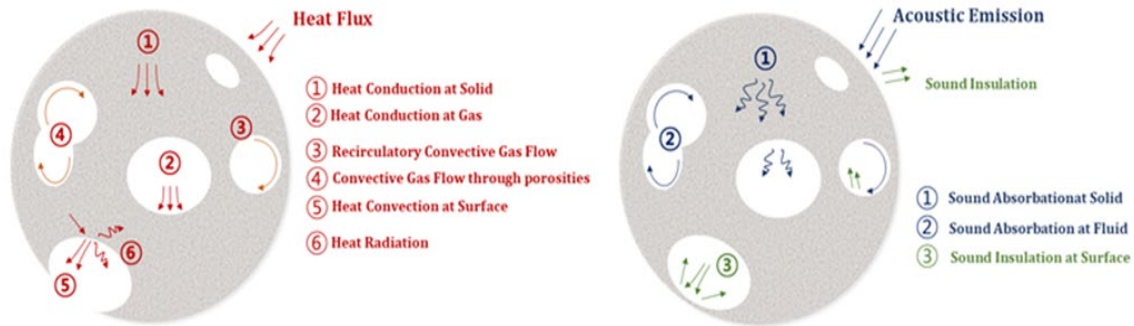


Figure1: Heat transfer and sound absorption mechanism in porous structure

Because the internal gas of porous structure can improve the thermal insulation and acoustic absorption properties, the application of the porous structure in building thermal insulation materials has attracted great attention[8]. Some simulation models about the thermal insulation and acoustic absorption mechanism in porous structures have been built[9-13]. Most of the porous structure in insulation materials is in the form of foam, and the Freon foaming agent used in conventional polymer do harm to the environment [14], however, additive manufacturing can design and produce porous structures which cannot be achieved with conventional foaming agents. Therefore, using additive manufacturing to develop heat insulation materials with functions of flame retardant, acoustic adsorption is of high significance.

Research contents and methology:

This goal of project is to develop an artificial intelligence-guided intelligent design system for fused deposition modeling (FDM) additive manufacturing technology, then based on this system, using FDM to manufacture a composite thermal insulation material with both flame-retardant and sound-absorbing functions.

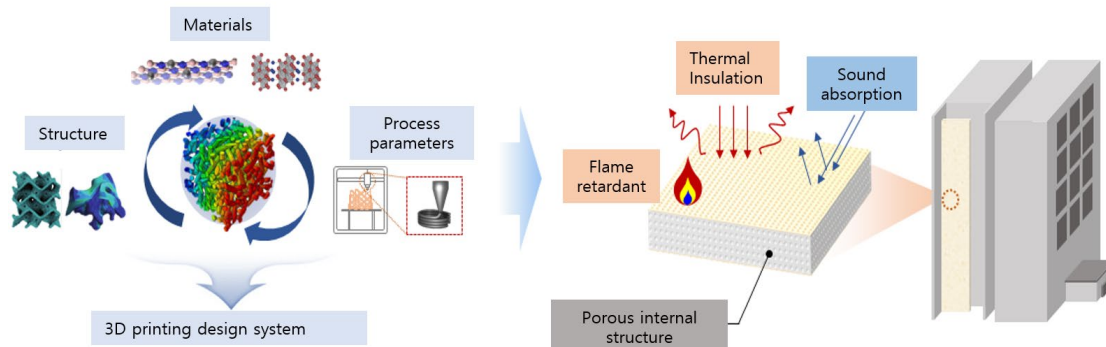


Figure2: The structure of the 3D printing system for developing thermal insulation, flame retardant and noisy adsorption materials.

The construction of database:

Generally, the data relate to the process parameters of FDM printer comes from the printing experiments, which means its size can not be huge. In that case, we can use Bayes regression, support vector machine to inference the optimal process parameters roughly. However, if the printing process can be simulated by software, we can use the simulation data to develop temporal neural networks, like recurrent neural networks (RNN).

There has been a lot of database about materials, but collecting useful data is still tricky for so many factors may affect the performance of the materials.

For the structure parameters, the data can be offered by simulation models. Generally we develop simulation models (like Finite element model, representational volume elements) firstly, then we can apply topology optimization or the Monte Carlo method on simulation models to develop the database.

Deep learning algorithms:

In most cases, the complexity of material design comes from spatial hierarchy and dynamic nature of materials. The spatial hierarchy is that for a multi-level structure, there is a strong interaction between levels and the interaction may be perfect or imperfect. The dynamic nature of materials means we have to take the time into consideration. For example, during the printing process, the temperature of material may change over time, and the temperature affect the property of printed part obviously. Therefore, we need deep learning algorithms which can describe the spatiotemporal hierarchy of materials. Convolutional neural network (CNN) can describe spatial distribution, and recurrent neural network (RNN) can describe the temporal distribution, hence, these two kinds of neural networks are most commonly used in material design.

For this project, we will develop FEM models which can simulate the mechanism of flame-retardant and sound-absorbing, then we will produce database based on these simulation models, finally CNN will be developed to replace these simulation models.

The CNN model we want to develop may be based on the ResUNet [17] (see Fig. 3a). It is a semantic segmentation neural network that based on residual learning and U-Net. By combining these two, it is possible to use the strengths of both. The network is built with residual units but uses a similar architecture to U-Net [17]. We hope to use this CNN model to find optimized structure parameters. The model will be trained using the above developed simulation database. U-Net is first proposed by Ronneberger et al. [18], it can improve segmentation accuracy by concatenating feature maps from different neural network levels. Here the main difference between the U-Net and the ResUNet is that the ResUNet uses residual units instead of neural units as the building block. The building block used in the conventional U-Net and the ResUNet has been shown in Fig. 3b and c respectively. As shown in Fig. 3c, ResUNet uses batch normalizations (BN), rectified linear units (ReLU), and convolutional layers (Conv), whereas shown in Fig. 3b,

U-Net uses ReLU and convolutional layers in the building block.

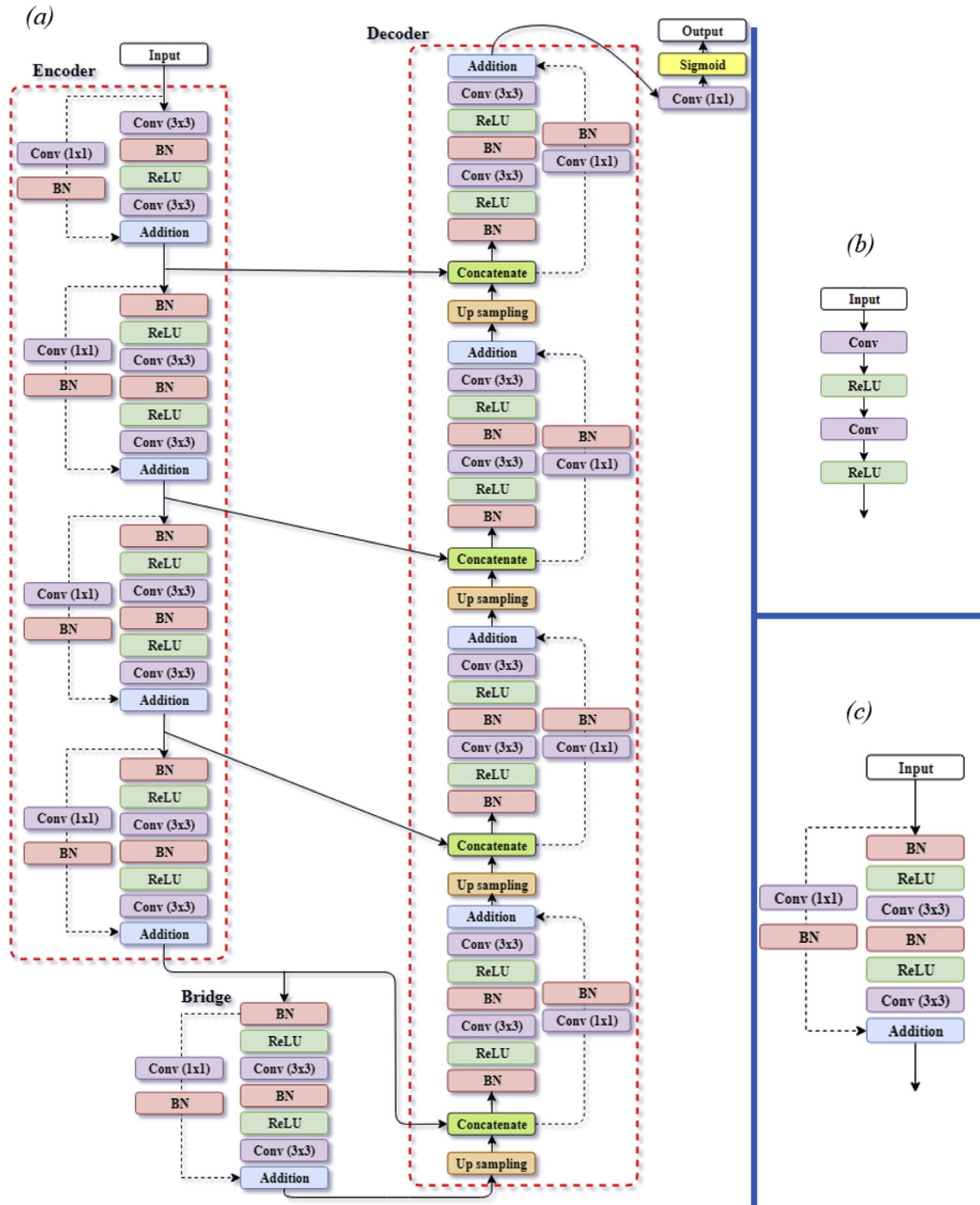


Figure 3: Illustration of the a) architecture of the ResUNet, b) building block used in U-net, and c) building block used in ResUNet.

Discussion:

Deep learning algorithms are the most popular techniques among artificial

intelligence technology. Because of its high design freedom, it can describe complex system. The hyperparameters of neural networks, like the number of hidden layers, connections among layers, sharing of model parameters among nodes, the choice of activation and loss functions, offer a huge design space. Generally, material design follows a system approach, for example, in this project, subsystems about flame retardant and sound-absorbing will be developed respectively by simulation. Using deep neural networks to replace these simulation models can save a lot of computation time, and make the coupling design efficient. All these prove that the development of deep learning can improve the efficiency of material design and further the wider application of additive manufacturing.

References:

- [1] 卢秉恒. 增材制造技术——现状与未来[J]. 中国机械工程, 2020, 31(01): 19-23.
- [2] Olson G B. Computational design of hierarchically structured materials[J]. Science, 1997, 277(5330): 1237-1242.
- [3] Shen C, Wang C, Wei X, et al. Physical metallurgy-guided machine learning and artificial intelligent design of ultrahigh-strength stainless steel[J]. Acta Materialia, 2019, 179: 201-214.
- [4] Yan W, Ge W, Qian Y, et al. Multi-physics modeling of single/multiple-track defect mechanisms in electron beam selective melting[J]. Acta Materialia, 2017, 134: 324-333.
- [5] Karpatne A, Atluri G, Faghmous J H, et al. Theory-guided data science: A new paradigm for scientific discovery from data[J]. IEEE Transactions on knowledge and data engineering, 2017, 29(10): 2318-2331.
- [6] Popova E, Rodgers T M, Gong X, et al. Process-structure linkages using a data science approach: application to simulated additive manufacturing data[J]. Integrating materials and manufacturing innovation, 2017, 6(1): 54-68.
- [7] Goh G D, Sing S L, Yeong W Y. A review on machine learning in 3D printing: Applications, potential, and challenges[J]. Artificial Intelligence Review, 2020: 1-32.
- [8] Abu-Jdayil B, Mourad A H, Hittini W, et al. Traditional, state-of-the-art and renewable thermal building insulation materials: An overview[J]. Construction and Building Materials, 2019, 214: 709-735.
- [9] Bracconi M, Ambrosetti M, Maestri M, et al. A fundamental analysis of the influence of the geometrical properties on the effective thermal conductivity of open-cell foams[J]. Chemical Engineering and Processing-Process Intensification, 2018, 129: 181-189.
- [10] Van De Walle W, Claes S, Janssen H. Implementation and validation of a 3D image-based prediction model for the thermal conductivity of cellular and granular porous building blocks[J]. Construction and Building Materials, 2018, 182: 427-440.
- [11] Mirabolghasemi A, Akbarzadeh A H, Rodrigue D, et al. Thermal conductivity of architected cellular metamaterials[J]. Acta Materialia, 2019, 174: 61-80.
- [12] Oh J H, Kim J S, Oh I K. Auxetic graphene oxide-porous foam for acoustic wave and shock energy dissipation[J]. Composites Part B: Engineering, 2020, 186: 107817.
- [13] Assouar B, Oudich M, Zhou X. Acoustic metamaterials for sound mitigation[J]. Comptes Rendus Physique, 2016, 17(5): 524-532.
- [14] Jin F L, Zhao M, Park M, et al. Recent trends of foaming in polymer processing: a review[J]. Polymers, 2019, 11(6): 953.
- [15] Duty C, Ajinjeru C, Kishore V, et al. What makes a material printable? A viscoelastic model for extrusion-based 3D printing of polymers[J]. Journal of Manufacturing Processes, 2018, 35: 526-537.
- [16] Zunger A. Inverse design in search of materials with target functionalities[J]. Nature Reviews Chemistry, 2018, 2(4): 1-16.
- [17] Zhang, Zhengxin, Qingjie Liu, and Yunhong Wang. "Road extraction by deep residual u-net." IEEE Geoscience and Remote Sensing Letters 15.5 (2018): 749-753.
- [18] Ronneberger, Olaf, Philipp Fischer, and Thomas Brox. "U-net: Convolutional networks for biomedical image segmentation." International Conference on Medical image computing and computer-assisted intervention. Springer, Cham, 2015.