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Developing GNN-based Surrogate Models for Multi-Objective Sustainable Performance Predictions of Residential Blocks

Zhaoji Wu [1], Wenli Liu [1], Jack C.P. Cheng [1], Zhe Wang [1], Helen H.L. Kwok [1], Cong Huang [1], and Fangli Hou [1]
[1] Department of Civil and Environmental Engineering, The Hong Kong University of Science and Technology, Hong Kong SAR
zwubz@connect.ust.hk, wliucd@connect.ust.hk, cejcheng@ust.hk, cezhewang@ust.hk, hlkwokab@connect.ust.hk, chuangax@connect.ust.hk, fhouaa@connect.ust.hk

Abstract

Although building performance simulation using physical models is frequently utilized for performance prediction, its significant computational demands pose challenges to its implementation in the early design stage. Surrogate models have been proposed to replicate computationally expensive physics-based simulation models, but existing surrogate models for sustainable residential block design are limited in scope, focusing on specific cases. Graph neural network (GNN) could be a solution to enhance the generality of the surrogate models for residential block design. However, the optimal architectures of the surrogate model and the time costs compared with physics-based simulation models have not been discussed yet. To fill these gaps, this study explores the development of GNN-based surrogate models for multi-objective sustainable performance predictions of residential blocks. Firstly, we introduce a graph schema to represent the general geometric features and relations, and a regional dataset for training and testing of the surrogate models. Secondly, we propose two kinds of architectures (individual architectures for specific indicators and an integrative architecture) for the surrogate models. Thirdly, we train and optimize the models utilizing the graph schema, regional dataset and architectures. Finally, the optimized surrogate models are evaluated in two aspects: 1) the optimized models using the individual architectures for specific indicators and the ones using the integrative architecture are compared in terms of prediction accuracy and time costs; and 2) the time costs of the optimized model are analyzed by comparing with physics-based simulations. The results showed that surrogate models based on individual architectures outperform the model using the integrative architecture in terms of prediction accuracy and time costs for all sustainable performance indicators. Although the model preparation time of the surrogate models exceeds that of the physics-based simulations, the surrogate models reduce the calculation time from 6.346 min to 1.565 ms per case compared with the physics-based simulations.

Keywords: Surrogate model, Graph neural network, Building performance prediction, Sustainable building design, Residential block

1 Introduction

The subject of sustainable design for residential blocks is progressively gaining significance within the realm of global urbanization and the escalating demand for ecologically conscious habitats. In 2022, residential energy consumption accounted for 20.96% of the total energy utilized in the building sector worldwide (International Energy Agency, 2023). Incorporating sustainable performance considerations during the initial design phase requires performance prediction, a fundamental process enabling the measurement of the level of sustainability achievable by designs. Building performance simulation using physical models is frequently utilized for performance prediction, such as structural and energy performance (Wong et al., 2023). However, its significant computational demands and time-intensive modeling pose challenges to its implementation in the early design phase (Attia et al., 2012). For example, in Natanian and Wortmann's study (Natanian & Wortmann, 2021), the time taken for full energy simulation using EnergyPlus for a nine-block district was 40 min and 30 s per iteration (500 iterations in total). The extended computational duration would not be viable during the initial design phase, where it is preferable for the feedback time of the program to remain under the threshold of 10 seconds. (Miller, 1968).

Surrogate models have been proposed to replicate computationally expensive physics-based simulation models (Westermann & Evins, 2019). Two studies (Hu et al., 2023; Wang et al., 2021) have developed surrogate models to predict multiple indicators of sustainable performance in the early design stage of residential buildings at block levels. These models offer substantial reductions in computational time (e.g., 500 times faster than physics-based simulation modeling (Z. Hu et al., 2023)), while preserving an acceptable level of accuracy during the optimization process in the early design stage. However, these surrogate models are based on artificial neural networks (ANNs) in which the input structures are fixed. Hence, the models are case-specific and cannot represent general residential block design.

A graph is a data structure representing a set of nodes interconnected by edges (Zhou et al., 2020) that has been introduced to the architecture, engineering and construction (AEC) industry (Jia, Wang, Shou, et al., 2023) (e.g., building energy simulation (Wu, Cheng, & Wang, 2023; Wu, Cheng, Wang, et al., 2023), generative design of sustainable buildings (Wu, Wang, et al., 2024a, 2024b), and compliance checking (Tao et al., 2024)). Graph neural networks (GNNs) are a class of neural networks specifically designed to operate on graph-structured data (Zhou et al., 2020) and have been adopted in surrogate models for building performance prediction (Y. Hu et al., 2022; Jia, Wang, Hosseini, et al., 2023; Lu et al., 2022). However, there is a lack of research examining GNN-based surrogate models in the context of sustainable residential block design. Using GNNs in surrogate models has two advantages, which may address the issues found in the current surrogate models for sustainable residential block design. Firstly, GNNs can not only consider the impacts from the building itself but also incorporate the influences from the surrounding buildings. Secondly, GNNs can handle inputs with varying numbers of nodes or edges without requiring extensive modifications to the network architecture, and hence GNNs can enhance the generality of surrogate models.

In our previous study (Wu, et al., 2024), we developed a surrogate model for multi-objective sustainable performance prediction based on GNN. Firstly, a graph schema is proposed to represent the general topological relations among components in residential block layout design. Secondly, a dataset is established based on parametric design models of residential blocks and simulations of sustainable performance, including energy consumption, daylighting, and thermal comfort. Finally, an architecture using graph attention network (GAT) is proposed for multiple sustainable performance predictions. The results showed that the proposed model (GAT) outperforms the benchmark models (GCN and ANN) in terms of prediction accuracy, indicating that the inclusion of neural networks with message passing mechanisms that consider the impact of surrounding buildings leads to accuracy improvement. However, this is the preliminary study exploring GNN-based surrogate models for sustainable residential block design. Two issues remain to be solved. For one thing, the current surrogate models for predicting multiple indicators of residential blocks (Z. Hu et al., 2023; Wang et al., 2021) were trained for each performance indicator individually. In contrast, in some studies on GNN-based prediction of multiple indicators (Li et al., 2023; Lu et al., 2022), one integrative model was trained for all the indicators. Consequently, when introducing GNN to the development of surrogate models for predicting multiple indicators of residential blocks, the adoption of architectures, the individual one or the integrative one, is an important issue to be addressed. For another, to facilitate smooth and efficient interaction between the designers and the simulation tool, the computational time needs to be short. However, the time costs of the GNN-based surrogate models for sustainable residential block design have not been discussed yet.

To solve these two issues, this study further explores the development of surrogate models for the early-stage design of residential blocks by leveraging GNN. Firstly, we introduce graph schema and regional dataset proposed the previous study (Wu et al., 2024). Secondly, we propose two kinds of architectures (individual architectures for specific indicators and an integrative architecture) for the GNN-based models. Thirdly, we train and optimize the GNN-based models utilizing the graph schema, regional dataset and architectures. Finally, the optimized surrogate models are evaluated in two aspects: 1) the optimized surrogate models using the individual architectures for specific indicators and the integrative architecture are compared in terms of prediction accuracy and time costs; and 2) the time costs of the optimized surrogate model are analyzed by comparing with physics-based simulations.

2 Method

2.1 Graph representation and dataset

A graph schema was developed to represent the general topological relations among components in residential block design (Wu et al., 2024). In the graph schema, nodes represent individual buildings within a residential zone and bi-directional edges represent positional relationships among the buildings. There is no edge connection between two buildings if these two buildings are completely obstructed by other buildings. Figure 1 shows the proposed graph model using one example of a residential zone with nine buildings. Nine nodes are used to represent the nine buildings. Bi-directional edges are established to represent the positional relationships among them, excluding buildings that are completely blocked by others (e.g., building 1 and building 3). The self-impact of a building on its sustainable performance is determined by building shape, building height, orientation, building volume, floor area, envelope area, window area, etc., while the impact of its surrounding buildings is determined by positional relationships (e.g., distances and relative angles) and obstructions between the two buildings. Accordingly, floor plan type, building height, window-to-wall ratio (WWR), north-south (N-S) projected length, west-east (W-E) projected length, shape factor and heat loss form factor are adopted as the node features, and relative angle, distance and visibility ratio are adopted as the edge features in the proposed graph schema.

The classification of floor plan types differs between regions. In this study, we take residential buildings in Hong Kong as an example and classify the floor plan type into six categories (Linear, L-shape, Y-shape, X-shape, Cruciform and Double-cruciform). To define the orientations of residential buildings, we introduce N-S projection length and W-E projection length to describe the building lengths along the north-south and west-east direction respectively (**Figure 2** (a)). In addition, the shape factor (or shape coefficient) (determined by Eq. (1)) (Depecker et al., 2001) and heat loss form factor (determined by Eq. (2)) (Andrew, 2021) are introduced as node features to incorporate the influence of building volume, floor area and envelope area.

$$SF = \frac{A_{envelope}}{V} \tag{1}$$

$$HLFF = \frac{A_{floor}}{A_{envelope}} \tag{2}$$

where SF is the shape factor, $HLFF$ is the heat loss form factor, V is the building volume, $A_{envelope}$ is the envelope area, and A_{floor} is the total floor area.

Figure 2 (b) defines the two edge features, distance and relative angle, which describe the positional relationships between two buildings. The centroids of the footprints of the two buildings are used to settle the distance and relative angle. To determine the obstruction conditions between two buildings, we propose a visibility ratio representing the portion of one building that can be "seen" by another. The visibility ratio is calculated by Eq. (3).

$$VP_{A\leftarrow B} = \frac{\sum_{i=1}^{M}\left(\frac{\sum_{j=1}^{N}\mathbb{1}(j\ is\ visible\ to\ i)}{N}\right)}{M}, \tag{3}$$

where $VP_{A\leftarrow B}$ is the visibility ratio from building B to A (the portion of B that A can "see"), i is the sampling point on the exterior surface of building A, j is the sampling point on the exterior surface of building B, M is the number of sampling points on building A, N is the number of sampling points on building B, and $\mathbb{1}(j\ is\ visible\ to\ i)$ is the indicator function that equates to 1 if there is no obstruction on the straight line from point j to point i, and 0 otherwise. **Figure 2** (c) is a visualization of the visibility ratio in which building C is the obstruction between building A and B, the red point is one of the sampling points on building A, and the area in grey represents the area visible to the red point. The grid size of the sampling points adopted in this study is 10 m.

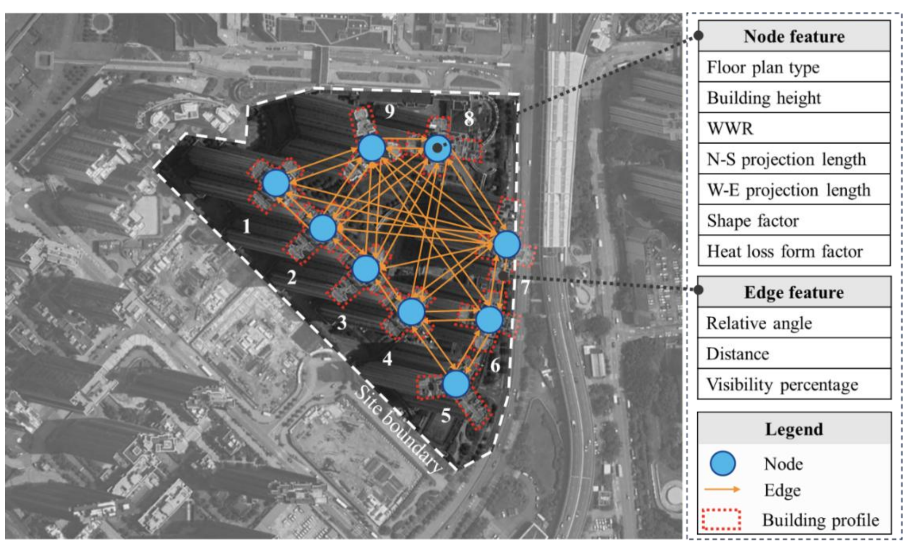
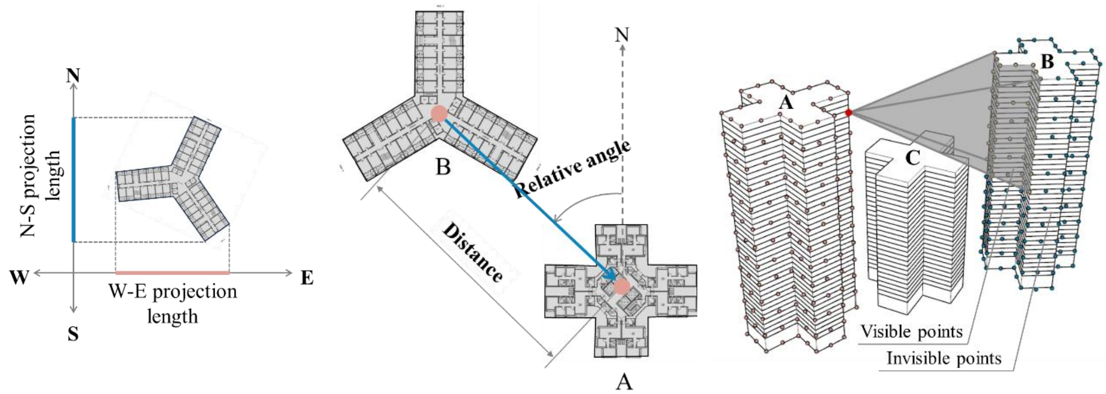


Figure 1: Graph representation of residential block layout design



(a) N-S projection length and W-E projection length

(b) Distance and relative angle from building B to A

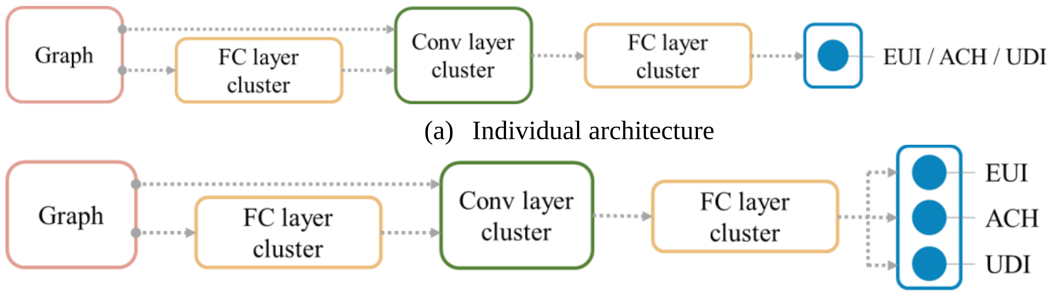
(c) Visibility ratio

Figure 2: Definitions of N-S projection length, W-E projection length, distance, relative angle and visibility ratio

To enhance the generality of the surrogate model for residential block design, it is essential to collect comprehensive data that spans an entire region, where shared common patterns or frameworks in the design of residential blocks exist. In the previous study (Wu et al., 2024), we took residential blocks of public housing in Hong Kong as an example to generate a dataset for the training and testing of the GNN-based surrogate models. The dataset was generated based on parametric design models and performance simulation, considering the schedules and behaviors (such as window opening for natural ventilation (Wu, Zhang, Mai, et al., 2023)) of the local residents. We used energy use intensity (EUI), annual comfort hours (ACH) and useful daylight illuminance (UDI) as the performance indicators of energy consumption, indoor thermal comfort and daylighting respectively. The dataset contains 9962 graphs, and each graph represents a residential zone, containing node features and performance indicators of each building and edge features. In this study, we introduce the dataset for the training and testing of the GNN-based surrogate models.

2.2 GNN architecture

We propose two kinds of architectures for our GNN-based surrogate models, individual architectures for specific indicators and an integrative architecture, as shown in Figure 3. The aim is to predict the sustainable performance indicators of each building in a residential zone, which is a node regression task (Zhou et al., 2020). The graphs containing node features and edge features of all the buildings serve as the inputs of the architecture. The main body of each architecture contains three parts: a first cluster of fully connected layers (FC layers) for pre-processing of the node features of the target building, a cluster of convolution layers (Conv layers) aggregating the edge features and node features from the target building itself and the surrounding buildings, and a second cluster of FC layers for post-processing after incorporating the information from the surroundings. In the individual architecture (Figure 3 (a)), the output only contains one performance indicator, and one model is trained for each of the performance indicators individually. In the integrative architecture (Figure 3 (b)), the outputs contain all the performance indicators, and one model is trained for all three performance indicators.



(b) Integrative architecture

Figure 3: The two kinds of adopted architectures for the GNN-based surrogate models

Figure 4 shows the detailed architecture for predicting multiple indicators of sustainable performance of residential blocks, using the integrative architecture as the example. GAT (Brody et al., 2021) is applied to the Conv layers and the GATv2 operator (PyG Team, 2024) is used to aggregate the node features and edge features from the target building and the surrounding buildings. In GAT, an attention mechanism is employed to assign different weights to the relations between nodes in a graph, which allows the network to focus on the most relevant nodes during information propagation. Multiple heads are also employed in GAT, which enables the network to capture complementary aspects of the graph structure. Each Conv layer is connected to an FC layer before passing data to the subsequent Conv layer. At the beginning of the first cluster of FC layers and the end of the second cluster of FC layers, the number of channels gradually increases and decreases (12 →n/2→n and n→n/2→3) respectively to ensure a smooth change of the number of channels. The rectified linear unit (ReLU) is adopted as the activation function except the last FC layer, where the Sigmoid function is used. The architectures are parameterized with five parameters, the number of neurons (n), the number of heads in GAT (h), the number of layers in the pre-processing FC layer cluster (N1), the number of layers in the Conv layer cluster (N2), and the number of layers in the post-processing FC layer cluster (N3).

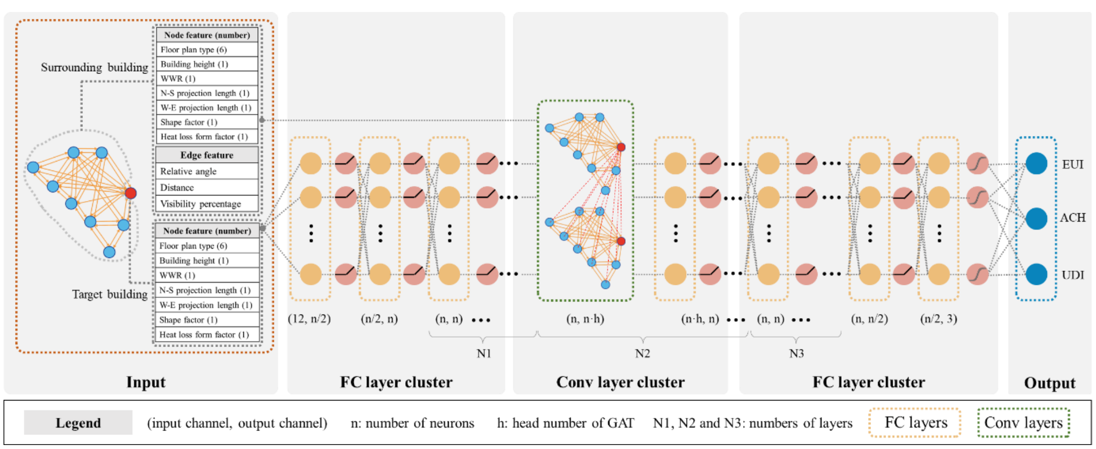


Figure 4: Details of the architecture (using the integrative architecture as the example)

2.3 Model training and evaluation

The dataset is randomly divided into a training set and a test set at the ratio of 75/25. The training data are then divided into smaller subsets and the model's parameters are updated based on the gradient computed from each mini-batch. Dropout is implemented to alleviate the overfitting issue.

The training uses Adam as the optimizer and MSE as the loss function. The architecture parameters are optimized first, and the hyper-parameters of the models with optimal architectures are optimized subsequently. In the cases with the individual architecture, the model that exhibits the lowest coefficient of variation of the root mean square error (CV(RMSE)) value for the performance indicator in the test set is considered the optimal model. In the cases with the integrative architecture, the optimal model is the one with the lowest average CV(RMSE) of the three performance indicators. Grid search is used to optimize the architecture parameters and hyper-parameters. The search spaces of the parameters are listed in Table 1. To evaluate the performance of the models, the mean absolute error (MAE), root mean square error (RMSE), and CV(RMSE) are introduced, as given in Eqs. (4)–(6).

$$MAE = \frac{1}{m}\sum_{i=1}^{m}|(y_i - \hat{y}_i)| \tag{4}$$

$$RMSE = \sqrt{\frac{1}{m}\sum_{i=1}^{m}(y_i - \hat{y}_i)^2} \tag{5}$$

$$CV(RMSE) = \sqrt{\frac{1}{m}\sum_{i=1}^{m}(y_i - \hat{y}_i)^2} \Big/ \frac{1}{m}\sum_{i=1}^{m}\hat{y}_i \tag{6}$$

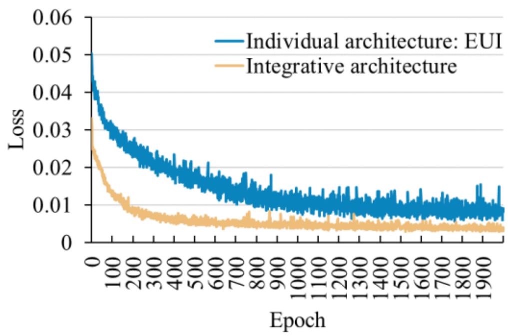
where m is the number of all predictions, y_i is the i^{th} prediction and $\hat{y}_i$ is the i^{th} ground truth.

The models are trained and tested using a desktop computer with the following specifications: Intel Core CPU i7–12700 at 2.10 GHz and 20 cores, NVIDIA GeForce RTX 3070 GPU, 32 GB RAM, and Windows 64 operating system. Python version 3.11.7, CUDA version 12.1 and PyTorch version 2.2.1 are used.

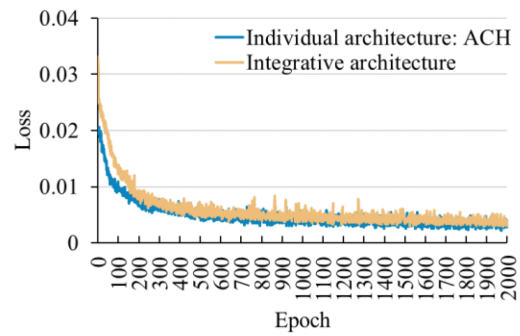
3 Results and discussion

3.1 Accuracy

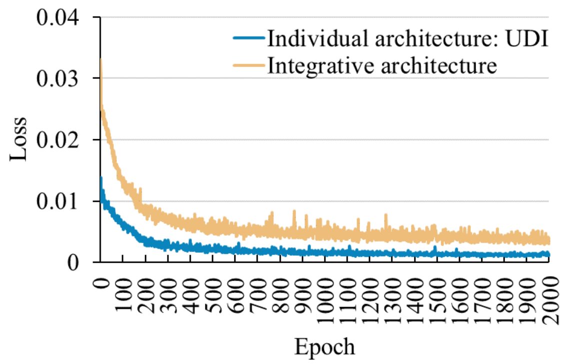
Figure 5 shows the loss curves of the training of the GNN-based surrogate models using different architectures. All models reach convergence within 2000 epochs during the training. The optimal parameters and the optimal architectures are shown in Table 1 and Figure 6 respectively. The optimal values of each hyper-parameter (batch size, learning rate and dropout) are the same among the different architectures in the search space used in this study. The optimal architectures for EUI and for ACH are similar, while the optimal architecture of UDI is different from the ones for EUI and for ACH. The different optimal architectures between EUI/ACH and UDI may result from the calculation mechanisms of the sustainable performance indicators. EUI and ACH are calculated based on thermodynamics while UDI is based on optics. Besides, although the optimal number of layers in the Conv layer cluster (N2), number of heads (h), number of layers in the pre-processing FC layer cluster (N1), and number of neurons (n) of the optimal individual architectures for EUI and for ACH are the same, the number of layers in the post-optimal processing FC layer cluster (N3) are different. The above result indicates that the calculations of EUI and ACH are similar in the pre-processing and the information aggregation, while the post-processing is different. Environmental parameters such as air temperature and relative humidity are calculated first based on thermodynamics for both EUI and ACH, while the thermal load is calculated for EUI and the thermal comfort index is calculated for ACH respectively later.



(a) EUI

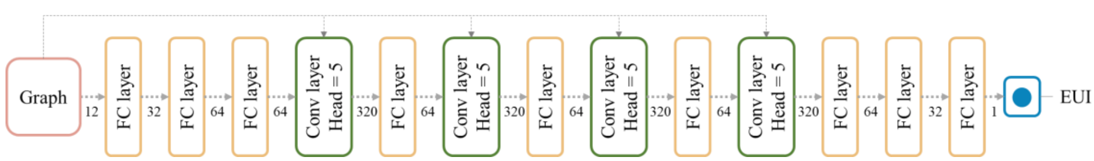


(b) ACH

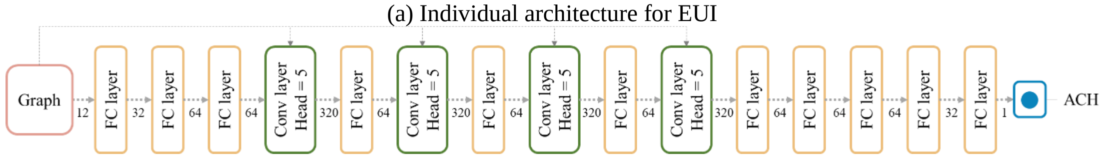


(c) UDI

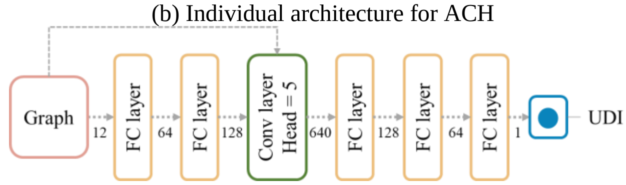
Figure 5: Loss curves of the training of the models using different architectures



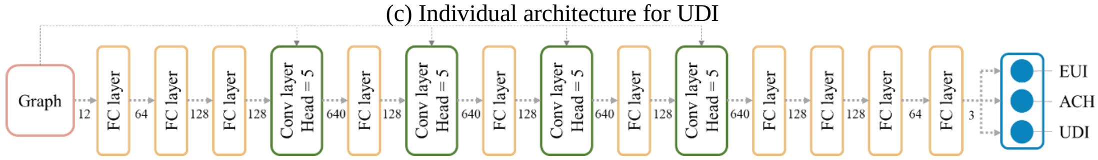
(a) Individual architecture for EUI



(b) Individual architecture for ACH



(c) Individual architecture for UDI



(d) Integrative architecture

Figure 6: Optimal architectures (the numbers of channels are listed under the arrows between two layers).

In addition, the number of Conv layers determine the depth of information aggregation, and the different optimal numbers of layers in the Conv layer cluster (N2) indicate the different information aggregation mechanisms among different sustainable performance. The optimal number of layers in the Conv layer cluster (N2) of the optimal individual architecture for UDI is one, showing that the daylighting performance of the target buildings is only impacted significantly by their 1-hop neighbors. In contrast, the optimal numbers of layers in the Conv layer cluster (N2) of the optimal individual architectures for EUI and for ACH are both four, showing that the thermal environment-related performance of the target buildings is impacted significantly by their 4-hop neighbors. According to the definition of edges in this study (Section 3.1), edge connections are established between two buildings only if those two buildings are not completely obstructed by other buildings. The daylighting performance of the target buildings is impacted by shading and daylight reflectance from the adjacent buildings that the target buildings can “see”. Thus, it is reasonable that the optimal individual architecture for UDI uses one Conv layer (i.e., only considering influence from 1-hop neighbors). In contrast, the thermal conditions of the target buildings may not only be affected by the buildings adjacent to the target buildings, but depend on the heat balance among a certain hop pf neighbors. Therefore, the optimal individual architectures for EUI and for ACH use multiple Conv layers, and 4-hop neighbors are considered to affect significantly on the target buildings.

Table 1: Optimal parameters of the individual architectures and the integrative architecture

Parameter	Search space	Optimal value			
		Individual architecture for EUI	Individual architecture for ACH	Individual architecture for UDI	Integrative architecture
Architecture parameter					
Number of layers in the Conv layer cluster (N2)	[1, 2, 3, 4, 5, 6]	4	4	1	4
Number of heads (h)	[1, 2, 3, 4, 5, 6]	5	5	5	5
Number of layers in the pre-processing FC layer cluster (N1)	[0, 1, 2, 3]	1	1	0	1
Number of layers in the post-processing FC layer cluster (N3)	[0, 1, 2, 3]	0	2	0	1
Number of neurons (n)	[32, 64, 128, 256, 512]	64	64	128	128
Hyper-parameter					
Batch size	[32, 64, 128, 256, 512]	256			
Learning rate	[0.0001, 0.0005, 0.001, 0.005, 0.01, 0.05, 0.1]	0.001			
Dropout	[0, 0.1, 0.2, 0.3, 0.4]	0.2			

Table 2 shows the prediction accuracy of the GNN-based surrogate models using different architectures. For each sustainable performance indicator, the surrogate model using the individual architecture outperforms the model using the integrative architecture, with smaller RMSEs and CV(RMSE)s on the test set. The difference in the prediction accuracy between the individual and the integrative architecture is minor for EUI (CV(RMSE) difference of 0.5% (|11.79%-11.85%| / 11.85%)), slightly higher for ACH (CV(RMSE) difference of 3.2% (|7.63%-7.88%| / 7.88%)), and largest for UDI (CV(RMSE) difference of 21.9% (|8.00%-10.14%| / 10.14%)). The optimal integrative architecture is close to the optimal individual architectures for EUI and for ACH, and is distinct from the optimal individual architecture for UDI, which accounts for the different prediction accuracy among the three performance indicators. During the model training, we use the minimal average CV(RMSE) of the three performance indicators as the optimization objective of the integrative architecture (Section 3.4). Therefore, the optimal result of the integrative architecture is a balance among the three performance indicators. The result shows that the balance tends to shift to the side of EUI and ACH. In the integrative architecture, the parameters of the model are shared by all the sustainable performance indicators, while the parameters in the models using the individual architectures are trained specifically for each sustainable performance indicator. Consequently, the prediction accuracy of the models using the individual architectures for specific indicators are higher than that of the model using the integrative architecture.

Table 2: Prediction accuracy using different architectures

	EUI			ACH			UDI		
	MAE	RMSE	CV(RMSE)	MAE	RMSE	CV(RMSE)	MAE	RMSE	CV(RMSE)
Training set									
Individual architecture	11.88	19.27	10.11%	1.41	2.17	5.48%	1.63	2.21	3.75%
Integrative architecture	9.65	16.42	8.62%	1.45	2.30	5.80%	3.59	5.71	9.69%
Test set									
Individual architecture	13.77	22.48	11.79%	1.86	3.01	7.63%	2.99	4.73	8.00%
Integrative architecture	12.98	22.60	11.85%	1.89	3.11	7.88%	3.83	5.99	10.14%

3.2 Time cost

Table 3 shows the training time of the GNN-based surrogate models using different architectures. For the individual architectures, the training time is proportional to the complexity of the models. The individual architecture for ACH has the largest complexity and hence takes the longest time to train. The total training time of the models using the individual architectures is 5,391 s while that of the model using the integrative architecture is 8,040 s. If the models using the individual architectures were trained in parallel, the training time could be reduced to 2,115 s (determined by the longest training time among the individual architectures). The total calculation time of the models using the individual architectures is 1.565 ms per case on average, while that of the model using the integrative architecture is 2.338 ms. Therefore, the individual architectures outperform the integrative architecture in terms of the time costs. If both the prediction accuracy and the time costs are considered, we can conclude that the individual architectures should be adopted over the integrative architecture when developing GNN-based surrogate models for predicting multiple indicators of sustainable performance in the early design stage of residential blocks.

Table 3 shows the time costs of the sustainable performance predictions using the surrogate models and the physics-based simulations. For the surrogate model-based prediction, the most time-consuming part is the model preparation. It takes approximately one day to manually develop the simulation models in the simulation software, while it takes more than 90 days to prepare the surrogate models (i.e., more than 90 times longer than the physics-based simulation modeling). However, the surrogate model-based method achieves a dramatically faster calculation speed than the physics-based simulation modeling by 243,297 times (from 6.346 min to 1.565 ms) and 104,062 times (from 6.346 min to 2.338 ms) when using the individual architectures and integrative architecture respectively. The calculation time of the surrogate models are within one second and hence the surrogate models are suitable for the early design stage, in which the acceptable feedback time should be less than 10 seconds (Miller, 1968).

Table 3: Time costs of indicator predictions using the surrogate models and the physics-based simulations.

	Surrogate model	Physics-based simulation
Model preparation	Dataset generation: ~90 d. Model training: <u>Individual architectures</u> EUI: 2,095 s, ACH: 2,115 s, UDI: 1,181 s, In total: 5,391 s. <u>Integrative architecture</u> 8,040 s.	Simulation modeling: ~ 1d.
Calculation (per case)	<u>Individual architecture</u> EUI: 0.410 ms, ACH: 0.751 ms, UDI: 0.404 ms, In total: 1.565 ms. <u>Integrative architecture</u> 2.338 ms.	EUI and ACH (using EnergyPlus): 4.479 min, UDI (using Radiance): 1.867 min, In total: 6.346 min.

4 Conclusions

In this study, we developed GNN-based surrogate models to predict multi-objective sustainable performance indicators for residential blocks. The research consisted of several key steps. We introduced graph schema and regional dataset proposed the previous study (Wu et al., 2024). We proposed two kinds of architectures (individual architectures for specific indicators and an integrative architecture) for the GNN-based models. Thirdly, we trained and optimized the GNN-based models utilizing the graph schema, regional dataset and architectures. Finally, the optimized surrogate models are evaluated in terms of accuracy and time costs.

The major findings of this study are summarized as follows.

- Surrogate models based on individual architectures outperform the model using the integrative architecture in terms of prediction accuracy and time costs for all sustainable performance indicators. Therefore, individual architectures are recommended for developing GNN models for predicting multiple performance indicators.
- Although the model preparation time of the surrogate models exceed that of the physics-based simulations, the surrogate models reduce the calculation time from 6.346 min to 1.565 ms per case compared with the physics-based simulations. This demonstrates that the GNN-based surrogate models can significantly accelerate the performance evaluation in the early design stage of residential blocks, and therefore facilitate a smoother performance-based design.

Some limitations have been identified and should be addressed in future studies.

- The dataset only includes buildings within a single residential zone, neglecting the potential impacts of surrounding buildings outside the site boundary. Future studies should incorporate these external factors that may affect buildings within the residential zone.
- This study focuses solely on three indoor sustainable performance metrics. Future studies should encompass a wider range of sustainable performance indicators, representing both indoor and outdoor environments.

References

Andrew, S. (2021, July 22). How to calculate form heat loss factor. - BuildPass. https://www.buildpass.co.uk/blog/how-to-calculate-form-heat-loss-factor/

Attia, S., Gratia, E., De Herde, A., & Hensen, J. L. (2012). Simulation-based decision support tool for early stages of zero-energy building design. Energy and Buildings, 49, 2–15.

Brody, S., Alon, U., & Yahav, E. (2021). How attentive are graph attention networks? arXiv Preprint arXiv:2105.14491.

Depecker, P., Menezo, C., Virgone, J., & Lepers, S. (2001). Design of buildings shape and energetic consumption. Building and Environment, 36(5), 627–635. https://doi.org/10.1016/S0360-1323(00)00044-5

Hu, Y., Cheng, X., Wang, S., Chen, J., Zhao, T., & Dai, E. (2022). Times series forecasting for urban building energy consumption based on graph convolutional network. Applied Energy, 307, 118231. https://doi.org/10.1016/j.apenergy.2021.118231

Hu, Z., Zhang, L., Shen, Q., Chen, X., Wang, W., & Li, K. (2023). An integrated framework for residential layout designs: Combining parametric modeling, neural networks, and multi-objective optimization for outdoor activity space optimization. Alexandria Engineering Journal, 80, 202–216. https://doi.org/10.1016/j.aej.2023.08.049

International Energy Agency. (2023). Buildings—Energy System—IEA. https://www.iea.org/energy-system/buildings

Jia, Y., Wang, J., Hosseini, M. R., Shou, W., Wu, P., & Chao, M. (2023). Temporal Graph Attention Network for Building Thermal Load Prediction. Energy and Buildings, 113507.

Jia, Y., Wang, J., Shou, W., Hosseini, M. R., & Bai, Y. (2023). Graph neural networks for construction applications. Automation in Construction, 154, 104984. https://doi.org/10.1016/j.autcon.2023.104984

Li, M., Liu, Y., Wong, B. C. L., Gan, V. J. L., & Cheng, J. C. P. (2023). Automated structural design optimization of steel reinforcement using graph neural network and exploratory genetic algorithms. Automation in Construction, 146, 104677. https://doi.org/10.1016/j.autcon.2022.104677

Lu, J., Zhang, C., Li, J., Zhao, Y., Qiu, W., Li, T., Zhou, K., & He, J. (2022). Graph convolutional networks-based method for estimating design loads of complex buildings in the preliminary design stage. Applied Energy, 322, 119478. https://doi.org/10.1016/j.apenergy.2022.119478

Miller, R. B. (1968). Response time in man-computer conversational transactions. Proceedings of the December 9-11, 1968, Fall Joint Computer Conference, Part I, 267–277.

Natanian, J., & Wortmann, T. (2021). Simplified evaluation metrics for generative energy-driven urban design: A morphological study of residential blocks in Tel Aviv. Energy and Buildings, 240, 110916. https://doi.org/10.1016/j.enbuild.2021.110916

PyG Team. (2024). torch_geometric.nn.conv.GATv2Conv—Pytorch_geometric documentation. https://pytorch-geometric.readthedocs.io/en/2.5.0/generated/torch_geometric.nn.conv.GATv2Conv.html#torch_geometric.nn.conv.GATv2Conv

Tao, X., Wu, Z., Xu, Y., Zheng, C., Fang, Y., Das, M., Liu, H., Gong, X., & Cheng, J. C. P. (2024). Smarter smart contracts for automatic BIM metadata compliance checking in blockchain-enabled common data environment. Advanced Engineering Informatics, 62, 102627. https://doi.org/10.1016/j.aei.2024.102627

Wang, S., Yi, Y. K., & Liu, N. (2021). Multi-objective optimization (MOO) for high-rise residential buildings' layout centered on daylight, visual, and outdoor thermal metrics in China. Building and Environment, 205, 108263. https://doi.org/10.1016/j.buildenv.2021.108263

Westermann, P., & Evins, R. (2019). Surrogate modelling for sustainable building design – A review. Energy and Buildings, 198, 170–186. https://doi.org/10.1016/j.enbuild.2019.05.057

Wong, B. C. L., Wu, Z., Gan, V. J. L., Chan, C. M., & Cheng, J. C. P. (2023). Parametric building information modelling and optimality criteria methods for automated multi-objective optimisation of structural and energy efficiency. Journal of Building Engineering, 75, 107068. https://doi.org/10.1016/j.jobe.2023.107068

Wu, Z., Cheng, J. C. P., & Wang, Z. (2023). An ontology-based framework for building energy simulation in the operation phase. Advances in Information Technology in Civil and Building Engineering, 351–366.

Wu, Z., Cheng, J. C. P., Wang, Z., & Kwok, H. H. L. (2023). An ontology-based framework for automatic building energy modeling with thermal zoning. Energy and Buildings, 296, 113267. https://doi.org/10.1016/j.enbuild.2023.113267

Wu, Z., Li, M., Liu, W., Wang, Z., Cheng, J. C. P., & Kwok, H. H. L. (2024, September 9). A data-driven model for sustainable performance prediction of residential block layout design using graph neural network. Proceedings of the 42nd Conference on Education and Research in Computer Aided Architectural Design in Europe (eCAADe 2024). The 42nd Conference on Education and Research in Computer Aided Architectural Design in Europe (eCAADe 2024), Nicosia, Cyprus.

Wu, Z., Wang, Z., Cheng, J. C. P., & Kwok, H. H. L. (2024a). A knowledge-informed optimization framework for performance-based generative design of sustainable buildings. Applied Energy, 367, 123318. https://doi.org/10.1016/j.apenergy.2024.123318

Wu, Z., Wang, Z., Cheng, J. C. P., & Kwok, H. H. L. (2024b, April 20). A knowledge graph model for performance-based generative design and its applications in accelerated design. Proceedings of The 29th Annual Conference for Computer-Aided Architectural Design Research in Asia (CAADRIA 2024).

Wu, Z., Zhang, Y., Mai, J., Wang, F., Zhai, Y., & Zhang, Z. (2023). Adaptation-based indoor environment control with night natural ventilation in autumn in an office building in a hot-humid area. Building and Environment, 243, 110702. https://doi.org/10.1016/j.buildenv.2023.110702

Zhou, J., Cui, G., Hu, S., Zhang, Z., Yang, C., Liu, Z., Wang, L., Li, C., & Sun, M. (2020). Graph neural networks: A review of methods and applications. AI Open, 1, 57–81. https://doi.org/10.1016/j.aiopen.2021.01.001