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Shangpeng Lei

PhD Student, Department of Computer Science
leishangpeng@foxmail.com, orcid.org/0009-0002-7156-4631
Al-Farabi Kazakh National University, Kazakhstan

Gulnur Balakayeva

Doctor of Physical and Mathematical Sciences, Department of Computer Science
gulnardtsa@gmail.com, orcid.org/0000-0001-9440-2171
Al-Farabi Kazakh National University, Kazakhstan

SPATIOTEMPORAL GRAPH PHYSICS-INFORMED NEURAL NETWORKS FOR DATA CENTER THERMAL MODELING

Abstract: Accurate thermal modeling is the precondition for improving energy efficiency and operational reliability of data centers (DCs). However, airflow circulation and workloads cause the temperature field of DCs to exhibit complex spatiotemporal variations. Conventional data-driven models formulate temperature prediction as a multivariate time-series task, without explicitly accounting for spatial heat interactions. In comparison, physics-based methods require detailed geometric information and high computational resources. To address these limitations, we propose a spatiotemporal graph physics-informed neural network (SGPINN) framework for multi-node and multi-step DC temperature prediction. Inspired by resistance-capacitance thermal modeling, SGPINN represents the thermal field as a graph, where graph aggregation captures spatial thermal interactions, and a physical residual combines temperature prediction with graph-guided thermal propagation. The temporal temperature derivative is obtained through automatic differentiation, while learnable equivalent thermal capacitance and heat-flow terms are introduced to characterize heterogeneous node dynamics without requiring directly measured physical parameters. A learnable multi-task strategy is adopted to adaptively balance the data loss and physics loss. The model is evaluated using both a real-world DC dataset and a simulated DC dataset and compared with four representative baseline models. SGPINN achieves the best overall performance on both datasets, with average MAEs of 0.1097 °C and 0.3043 °C, respectively. In the real-world case, it reduces average MAE and RMSE by 3.57% and 3.58% compared with APINN, while ablation results verify the contributions of graph modeling, physical constraints, and adaptive loss weighting. These findings suggest that SGPINN improves predictive accuracy while providing a physics-guided framework for DC thermal modeling.

Keywords: physics-informed machine learning, data center, thermal modeling, predication

Introduction

In recent years, the rapid development of cloud computing and artificial intelligence (AI) has greatly expanded the scale of digital services, and data centers (DCs) have become a key component of modern infrastructure [1,2]. Therefore, the computational demand has been increasing steadily, which accounts for approximately 3% of global electricity use [3]. Most of the electricity is transformed into heat, which causes the thermal accumulation and localized hot spots, degrading equipment performance [4]. To ensure the continuous operation of DCs, effective cooling is necessary to offer a stable thermal environment. Accurate thermal modeling provides an essential basis for characterizing the spatiotemporal evolution of temperature fields, improving cooling efficiency, and ensuring the reliable operation of DCs.

The thermal behavior of DC is complex to capture, including spatiotemporal interactions and nonlinear variation [5]. Heat generation of servers varies with computational demand, cooling-system operation, and airflow organization. Meanwhile, the heat propagation of DC follows physically meaningful paths that involve cold-air supply, heat exchange around server racks, and hot-air recirculation. These characteristics distinguish DC temperature fields from conventional multivariate

time-series data. The temperature evolution depends on both temporal history and the thermal states of neighboring locations. Therefore, an effective thermal modeling method should capture both temporal dynamics and spatial heat propagation while preserving the underlying physical consistency of DC.

Traditional physical simulation methods (PS) [6-7] used for DCs thermal analysis provided interpretable descriptions of thermal behavior, but they are limited by detailed setting and computational costs. The flexibility of PS methods is constrained when the DC layout, or cooling strategy changes. In comparison, data driven methods (DD) learn complex nonlinear mappings directly from observed data [8-9]. Nevertheless, purely DD models typically formulate temperature prediction as a sequential task without explicitly modeling of the heat physical propagation of DC.

To overcome the limitations of both PS and DD modeling, hybrid methods combine PS with DC in a relatively direct manner, such as simulated data for modeling [10], integrating automated simulation workflows with ML [11]. Although hybrid methods improve the usability of PS and DD methods, the coupling between physics and data is often external or sequential, while the model learning process is not constrained by physical principles. Different from loosely coupled hybrid strategies, physics informed machine learning (PIML) embeds physical knowledge into the learning process [12], such as physical loss functions, physics guided network architectures and physical feature representations to guide or constrain the learning process. An adaptive physics consistent neural network (A-PINN) [13] has been proposed, demonstrating the successful application of PIML for DC thermal modeling. Existing DC modeling methods have made important progress. However, there remains to work for improvement in simultaneously adaptive learning and spatiotemporal modeling. Graph neural networks (GNNs) provide a promising solution for modeling DC temperature fields. The behaviors of DC can be well represented with graph components, when we treat different locations as nodes, and thermal interaction as edges. As a result, GNNs explicitly represent the spatial interaction relationships among different thermal regions through message passing.

To capture thermal evolutionary distribution of DC, we propose a spatiotemporal graph physics-informed neural network (SGPINN), inspired by resistance-capacity modeling. The temporal derivative of temperature is computed through the automatic differentiation mechanism of the neural network (NN). The physical constraint is formulated by evaluating the residual between the NN approximated heat flow propagation and the thermal variation derived from the temporal temperature derivative. A multi task learning strategy is adopted to adaptively balance the thermal capacitance term and the physical loss. The model performs recursive multi step prediction and is evaluated on both real world and simulated datasets. The main contributions are listed as follows:

- We propose a SGPINN method for DC thermal modeling, predicting multi-node temperature with heterogeneous thermal dynamics, to combine the data relevance with physical intuition in modeling process.
- We design a physical consistency mechanism by combining the automatically differentiated temperature with a learnable node heat capacity and incorporating thermal propagation with NN.
- We evaluate proposed framework on real-world and simulation dataset, and compared with other advanced baselines in multi-step predictions, comprehensively demonstrating the generalization and effectiveness.

Materials and methods

To comprehensively evaluate the proposed method, two datasets were collected, including a real-world DC dataset and a simulation dataset developed in this study. Both datasets were split chronologically into the first 80% for training, the next 10% for validation, and the final 10% for testing. The real-world dataset contained 44,640 samples, and the simulated dataset contained 7,200 samples.

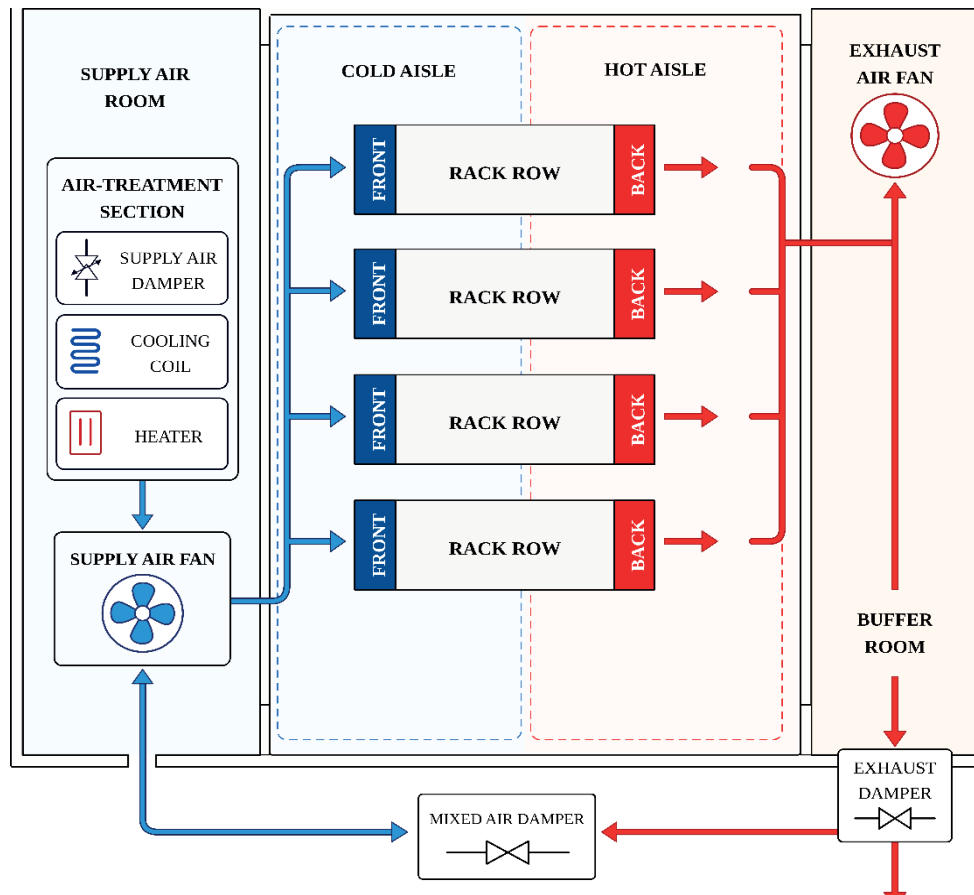


Figure 1 – The layout of real-world DC

The real-world dataset is from 17:00 on 31 July 2019 to 16:59 on 31 August 2019 with interval of 1 min, collected in a public DC in Singapore [14]. This DC has four server racks where ten points located in the cold aisle, the hot aisle, and the inlet and outlet of the racks. The thermal propagation of DC is dominated by the airflow organization. Specifically, mixed cold air is supplied at the cold aisle, then the heat generated by the servers are removed by the air flowing, finally the cumulative heat is gathered in hot aisle through the rack outlets. The layout of real-world DC is shown in Figure 1.

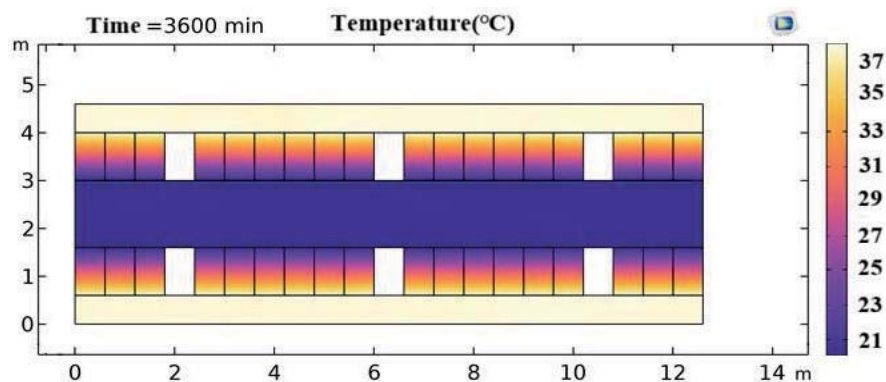


Figure 2 – Temperature distribution in simulation case at middle time

The simulated dataset was computed based on a two-dimensional large space, multi-rack DC configuration, whose geometric parameters were designed with reference to a representative thermal modeling case [15]. The simulated case is an in-row DC, and the cold aisle is located in the middle and the hot aisles are arranged on both sides. There are 36 server racks that the width and length of each rack is 0.60 m and 1.00 m, respectively. Since this research focuses on the thermal distribution

of the DC rather than the detailed internal flow inside the racks, we simplified the rack interiors as porous media. An inflow velocity is 2 m/s at the rack inlet, and the supply air temperature is 20 °C. The outlet boundary is a pressure condition with backflow suppression. To simulate realistic operating conditions, a time varying heat load is designed with reference to the M shaped demand response curve of DC [16]. The heat load varies between 2 kW and 4.5 kW with two daily peak periods occurring at 10:00 and 15:00. The size of simulated dataset is five-day period with a interval of 1 min. Figure 2 shows the distribution of simulated DC in the middle time.

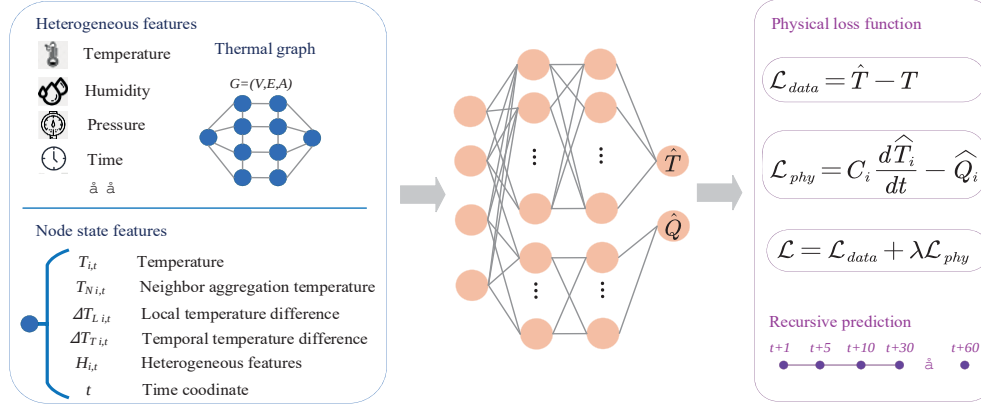


Figure 3 – The framework of SGPINN for DC thermal modeling

As shown in Figure 3, the DC thermal field is modeled with a graph data structure. The spatial thermal interaction among nodes is constrained by a normalized adjacency matrix. To clarify the thermal transmission, a correlation matrix computed based the temperature sequence. The Pearson correlation coefficient was calculated between each pair of node temperature sequences.

$$P_i = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^n (x_i - \bar{x})^2} \sqrt{\sum_{i=1}^n (y_i - \bar{y})^2}}, \quad (1)$$

where x and y denote the temperature sequences in different nodes.

The absolute correlation value was used to measure the thermal association, and these correlations were calculated using only the training set. The top 3 nodes with the largest absolute correlation values were selected as correlated neighbors, while the diagonal elements were set to zero. Therefore, the adjacency matrix represents whether two nodes exhibit strong temperature correlation rather than physical topology. For graph aggregation, self-loops are used to preserve node thermal state. The matrix is then normalized by row so that the weights associated with each node sum to one. In this formulation, the original adjacency matrix defines the topology of thermal correlations, whereas the adjacency matrix constructs the spatial propagation for thermal information. At each time step, the historical multi-node observations are used as model inputs. The graph structure is used to construct physically meaningful node thermal states $S_{i,t}$.

$$T_{N,i,t} = \frac{1}{n} \sum_{j=1}^n T_{j,t}, \quad (2)$$

$$\Delta T_{L,i,t} = T_{i,t} - T_{N,i,t}, \quad (3)$$

$$\Delta T_{T,i,t} = T_{i,t} - T_{i,t-1}, \quad (4)$$

$$H_{i,t} = \text{MLP}(F_{i,t}), \quad (5)$$

$$S_{i,t} = \{T_{i,t}, T_{N,i,t}, \Delta T_{L,i,t}, \Delta T_{T,i,t}, H_{i,t}, t\}, \quad (6)$$

where $T_{j,t}$ denotes the temperature of j - th node at t - th time. n denotes the number of neighbors. $F_{i,t}$ denotes the features except temperature, such as humidity and pressure. MLP is multilayer perceptron model.

Resistance-capacity thermal model (RC model) [17-18] provides a classical reduced order approach for describing transient heat transfer processes. The basic idea is derived from the electro thermal analogy, where temperature is regarded as voltage, heat flow is analogous to electric current. Thus, thermal resistance represents the difficulty of heat transfer between two nodes, and thermal capacity characterizes the heat storage capacity of a thermal mass. By lumping a distributed thermal field into several representative nodes, the dynamic temperature evolution can be expressed by energy balance equations. For a thermal node, a typical RC formulation can be written as follows:

$$C_i \frac{dT_i}{dt} = \sum_j^n \frac{T_j - T_i}{R_{j,i}} + \sum_k^K q_{i,k}, \quad (7)$$

where T_i denotes the i - th node, C_i denotes equivalent thermal capacity of i - th node, $R_{j,i}$ denotes the equivalent thermal resistance between the i - th node and the j - th node, and q_k denotes the k - th direct heat input of i - th node. Compared with full order numerical simulations, such as CFD or finite element models, RC networks retain the main energy balance relationship while greatly reducing computational complexity. Therefore, they are widely used in building energy modeling [19], HVAC control [20] and DC thermal modeling [21-22]. However, conventional RC networks usually rely on simplified topology, predefined thermal nodes, and identifiable physical parameters, which may limit their ability to represent complex airflow induced heat propagation and heterogeneous spatiotemporal interactions in modern data centers. This limitation motivates us to integrate RC model with graph, where thermal nodes and heat transfer paths can be represented as graph structures and learned from operational data.

Considering the generalization, we regard $\sum_j^n \frac{T_j - T_i}{R_{j,i}}$ and $\sum_k^K q_{i,k}$ as an integration term Q_i . Consequently, the Equation (7) can be transformed as follows:

$$C_i \frac{dT_i}{dt} = Q_i, \quad (8)$$

where the $\frac{dT_i}{dt}$ is obtained by automatic differentiation of neural network, C_i is a learnable positive parameter for each node, and Q_i is a learnable parameter without positive limitation. To further explain, the C_i is constrained to be positive through a Softplus transformation, whereas q_i is unconstrained so that it can represent net heat absorption or release. Because neither term is derived from material measured, their numerical values do not refer specific physical units. Moreover, the residual permits compensating scaling of C_i and q_i , so the two terms are not identifiable as physical parameters. Here, we interpret them as RC inspired equivalent latent coefficients that regularize the learned temperature dynamics. Their spatial variation can be referred as a model thermal indicator, but not as a direct estimation of thermal capacitance or heat flow.

Based on $S_{i,t}$, two coupled node MLP heads are used to model the data integrated graph information. One of MLP head predicts the temperature of each node, while another head estimates the corresponding heat flow term. These two outputs are coupled through a residual of Equation (8).

$$\mathcal{L}_{data} = \frac{1}{N} \sum_i^N (\hat{T}_i - T_i)^2, \quad (9)$$

$$\mathcal{L}_{phy} = \frac{1}{N} \sum_i^N (C_i \frac{d\hat{T}_i}{dt} - Q_i)^2, \quad (10)$$

$$\mathcal{L} = \mathcal{L}_{data} + \lambda \mathcal{L}_{phy}. \quad (11)$$

The total training objective consists of the data loss and the physical residual loss, balanced by a learnable coefficient constrained within $[0,1]$. The results were evaluated with three metrics, mean absolute error (MAE), root mean square error (RMSE), and coefficient of determination (R^2). These metrics are defined as follows:

$$\text{MAE} = \frac{1}{n} \sum_{i=1}^n |y_i - \hat{y}_i|, \quad (12)$$

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{n}}, \quad (13)$$

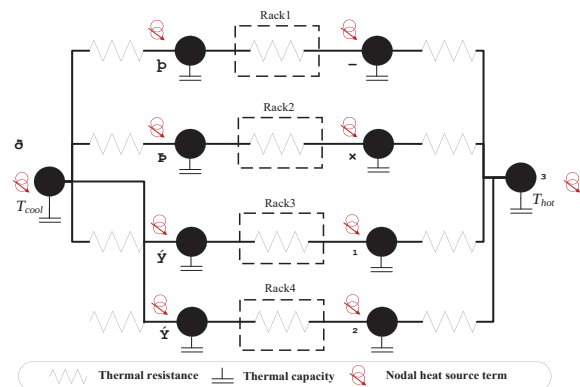
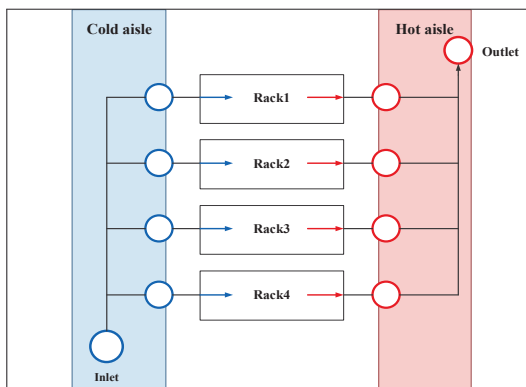
$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2}, \quad (14)$$

where y_i and $\hat{y}_i$ denote the observed and predicted values, respectively, $\bar{y}$ is the mean of the observed values, and n represents the total number of evaluated prediction points.

To ensure a fair comparison, all models were trained on the same data in PyTorch. The SGPINN used a window with the length of 12-minute as input, and recursively evaluated at forecasting horizons of 1, 5, 10, 30, and 60 min. For the real-world dataset, the available auxiliary variables were standardized using Z-score normalization [23], with the mean and standard deviation estimated exclusively from the training set and then applied unchanged to the validation and test subsets, while temperature was retained in the original values. The model was optimized using Adam with a batch size of 64, a learning rate of 10^{-3} , and a maximum of 100 epochs. The early-stopping checkpoint keeps the lowest validation mean squared error (MSE), and training was stopped if the validation MSE did not improve for 10 consecutive epochs. All baseline adopted as the same as the hyperparameter as the SGPINN.

The SGPINN consists two prediction heads. The prediction head has two hidden layers with 16 neurons, and heat flow estimation head has single layer with 8 neurons. The two heads were jointly optimized through the data loss and the physical residual loss. For comparison, four baseline models were implemented, which are APINN [13], EV-LSTM [9], standard spatiotemporal graph neural network (SSGNN), and Transformer. All model were used two hidden layers with 16 neurons architecture.

Results and discussion



(a) Physical layout of real-world

(b) The RC model of real-world case

Figure 4 – The topology model of real-world case

As shown in Figure 4, the real-world case can be topologically represented as a graph network with 10 nodes using RC modeling.

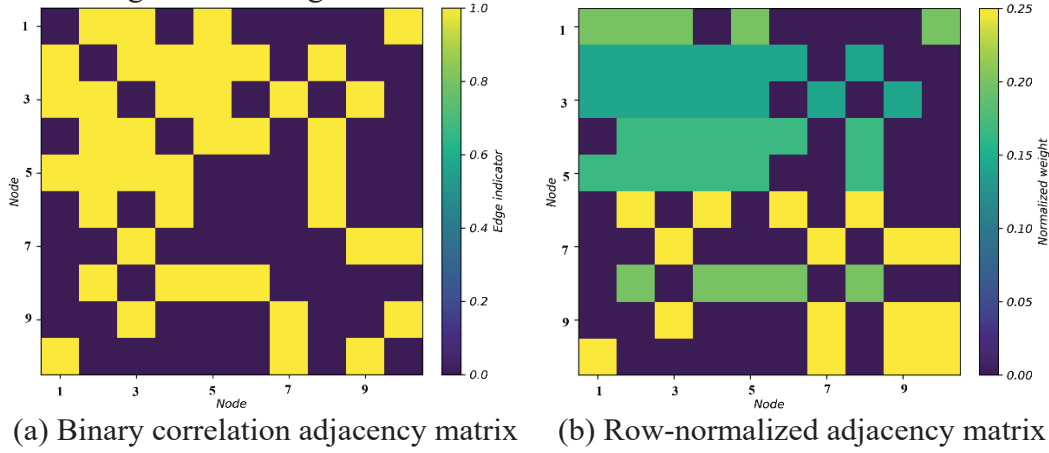


Figure 5 – The adjacency matrix results of real-world case

Figure 5 presents the binary correlation adjacency matrix and row-normalized matrix used for graph guided thermal state construction. As shown in Figure 5(a), yellow color indicates that two nodes were selected as strongly correlated thermal neighbors, while dark color suggests the absence of correlation. The heatmap exhibits a heterogeneous pattern rather than a regular topology, which is physically reasonable as nodes located in similar thermal regions tend to exhibit correlated temperature variations. Figure 5(b) shows the adjacency matrix, where the color intensity represents the relative contribution of each node in aggregation. It suggests graph correlations, which captures thermal variation that may be influenced by control strategy coupled heat propagation.

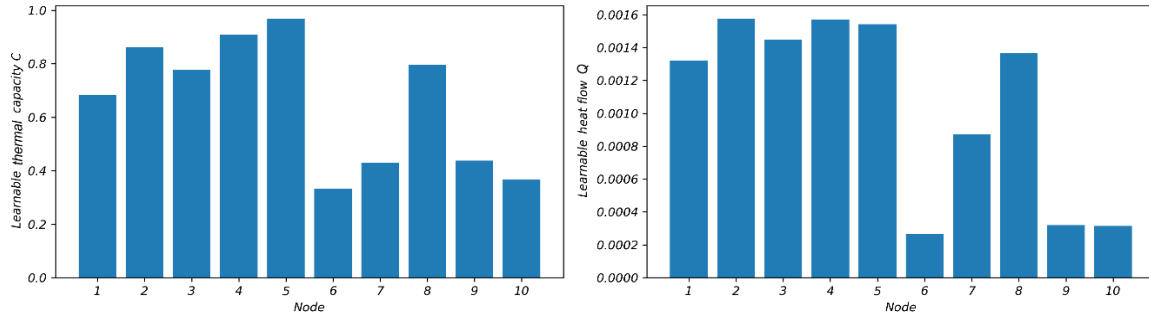


Figure 6 – The learnable equivalent terms of nodes in real-world case

It should be noted that the learned equivalent thermal capacitance and heat flow are not strictly defined physical terms. Instead, they are equivalent terms inspired by the physical principles within the data-driven framework. The learned equivalent thermal capacitance and heat flow terms exhibit clear spatial heterogeneity across the thermal topology. Nodes 2–5 show relatively large values of both C and Q , indicating that these nodes dominate in thermal storage and heat exchange. Node 7, 8 also presents a relatively high values, as their location are rack downstream with intensive interaction. These results demonstrate that the learned RC terms are topology related.

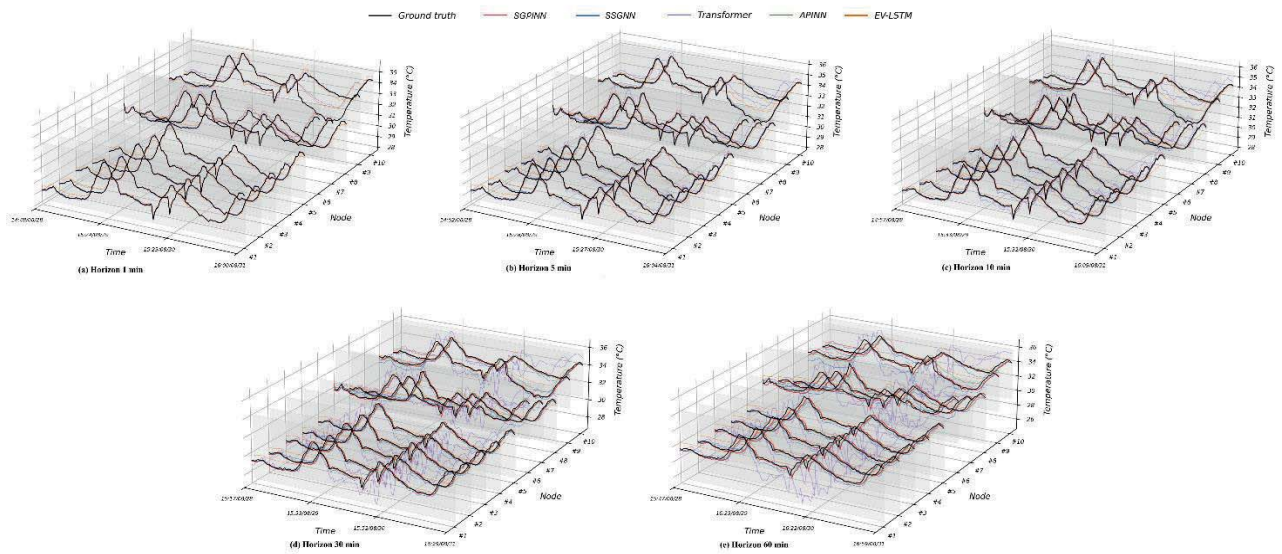


Figure 7 – The real-world temperature prediction result at different horizon

As shown in Figure 7, the errors of all models exhibit a gradual increase with the prediction horizon changing. For short-term prediction tasks, most models can follow the ground truth trajectories. However, for medium-long-term horizons, topology aware models show clear advantages. SGPINN usually agrees with the ground truth, preserving both the temporal trend and the spatial thermal pattern. In contrast, Transformer and EV-LSTM show unsatisfactorily in local extreme value. APINN predicts physically stably but more conservative in sharp thermal fluctuations. These observations suggest that explicitly incorporating the thermal topology and graph heat propagation mechanism is effective for temperature field prediction in DC.

Table 1 – The evaluation metrics of real-world case

Method	Horizon(min)	MAE	RMSE	R ²	Average		
					MAE	RMSE	R ²
SGPINN	1	0.0180	0.0250	0.9998	0.1097	0.1520	0.9859
	5	0.0501	0.0696	0.9981			
	10	0.0750	0.1059	0.9957			
	30	0.1564	0.2166	0.9821			
	60	0.2488	0.3428	0.9536			
SSGNN	1	0.0250	0.0330	0.9996	0.1786	0.2216	0.9683
	5	0.0661	0.0866	0.9971			
	10	0.1081	0.1393	0.9926			
	30	0.2550	0.3126	0.9626			
	60	0.4389	0.5366	0.8895			
APINN	1	0.0185	0.0253	0.9998	0.1138	0.1577	0.9853
	5	0.0537	0.0730	0.9980			
	10	0.0814	0.1136	0.9951			
	30	0.1638	0.2304	0.9797			
	60	0.2515	0.3464	0.9541			
EV-LSTM	1	0.2206	0.3047	0.9644	0.3419	0.4335	0.9226
	5	0.2922	0.3675	0.9482			
	10	0.2754	0.3675	0.9482			
	30	0.3916	0.4896	0.9083			
	60	0.5297	0.6380	0.8441			
Transformer	1	0.1384	0.2615	0.9738	0.6159	0.8332	0.7662
	5	0.2314	0.3565	0.9513			

	10	0.3393	0.4781	0.9124			
	30	0.8618	1.1115	0.5273			
	60	1.5086	1.9583	0.4662			

Table 1 reports the prediction performance of different models on the real-world DC case. Compared with SSGNN, SGPINN reduces MAE and RMSE by 38.58% and 31.37%, respectively, which suggests that the topology aware thermal modeling can more effectively capture the spatial heat interactions. SGPINN reduces MAE and RMSE by 3.57% and 3.58% than APINN, respectively. This suggests that the thermal graph is benefit to capture spatiotemporal evolution dynamics. In contrast, EV-LSTM and Transformer show substantially larger errors. SGPINN reduces MAE by 67.88% and 82.19% compared with EV-LSTM and Transformer, respectively. These results demonstrate that temporal recurrent modeling or sequential attention modeling is insufficient for accurately representing the airflow driven thermal dynamics in real-world DCs.

Table 2 shows the prediction performance of different models on the simulation case. SGPINN also achieves the best overall performance. From the real-world case to the simulation case, the absolute errors of most models increase, which can be attributed to the wider spatial variation and less data size in the simulation scenario.

Table 2 – The evaluation metrics of simulation case

Method	Horizon(min)	MAE	RMSE	R ²	Average		
					MAE	RMSE	R ²
SGPINN	1	0.0206	0.0286	0.9998	0.3043	0.4646	0.9903
	5	0.0729	0.1068	0.9998			
	10	0.1436	0.2135	0.9991			
	30	0.4272	0.6402	0.9915			
	60	0.8572	1.3339	0.9611			
SSGNN	1	0.0384	0.0562	0.9999	0.3436	0.5572	0.9872
	5	0.1089	0.1662	0.9995			
	10	0.1886	0.2916	0.9983			
	30	0.4872	0.7845	0.9873			
	60	0.8951	1.4876	0.9510			
APINN	1	0.0236	0.0319	0.9998	0.3597	0.5191	0.9883
	5	0.0942	0.1309	0.9997			
	10	0.1821	0.2554	0.9987			
	30	0.5159	0.7395	0.9887			
	60	0.9827	1.4380	0.9546			
EV-LSTM	1	1.2589	1.4003	0.9615	1.5809	1.9894	0.9165
	5	1.6171	1.9069	0.9281			
	10	1.7976	2.4634	0.8790			
	30	1.4981	2.1240	0.9067			
	60	1.7328	2.0525	0.9072			
Transformer	1	0.0542	0.0648	0.9999	0.3186	0.5437	0.9895
	5	0.1549	0.2217	0.9990			
	10	0.2333	0.3650	0.9973			
	30	0.4258	0.7931	0.9870			
	60	0.7248	1.2739	0.9643			

The improvement over EV-LSTM is particularly significant in both cases, confirming that purely temporal recurrent modeling is insufficient for representing spatially coupled thermal dynamics. Meanwhile, Transformer performs poorly in the real-world case but becomes competitive

in the simulation case, suggesting that attention temporal modeling can be benefit from more regular and smoother temperature, but lacks sufficient physical inductive bias when dealing with noisy real-world thermal DC. It is also worth noting that APINN performs competitively in the real-world case, with only slightly higher errors than SGINN. However, in the simulation case, its error increases more evidently, which suggests that physical constraints are not sufficient to fully characterize heat propagation despite improving prediction stability.

To clarify the contribution of the graph component, physics loss, and learnable weighting, the ablation experiments were conducted.

Table 4– The setting of ablation experiments

Variants	Graph	Physics loss	Loss weight
SGPINN	✓	✓	✓
#1 (no graph)	×	✓	✓
#2 (no physics term)	✓	×	×
#3 (fixed weight)	✓	✓	$\lambda = 0.5$

As shown in Table 5, removing the graph component increased the average MAE and RMSE to 0.1652 and 0.2100, respectively, corresponding to increases of 48.2% and 38.9% over the complete model. Removing the physical term makes an MAE of 0.1386 and an RMSE of 0.1946, whereas replacing learnable weighting with a fixed coefficient ($\lambda = 0.5$) produced values of 0.1498 and 0.2023. The corresponding R^2 values decreased to 0.9738, 0.9771, and 0.9753.

Table 5 – The results of ablation experiments

Method	Horizon(min)	MAE	RMSE	R^2	Average		
					MAE	RMSE	R^2
#1	1	0.0246	0.0478	0.9991	0.1652	0.2100	0.9738
	5	0.0762	0.0833	0.9973			
	10	0.0968	0.1456	0.9919			
	30	0.2342	0.3042	0.9646			
	60	0.3942	0.4691	0.9159			
#2	1	0.0232	0.0311	0.9996	0.1386	0.1946	0.9771
	5	0.0748	0.0763	0.9978			
	10	0.0902	0.1388	0.9926			
	30	0.1893	0.2943	0.9669			
	60	0.3154	0.4323	0.9286			
#3	1	0.0237	0.0382	0.9994	0.1498	0.2023	0.9753
	5	0.0753	0.0802	0.9975			
	10	0.0932	0.1401	0.9925			
	30	0.2193	0.2992	0.9657			
	60	0.3376	0.4539	0.9213			

Conclusion

This study proposed a SGPINN for DC thermal modeling. By combining graph thermal aggregation with physical residual, the framework captures both data driven spatiotemporal patterns and physical heat propagation characteristics. The proposed method was evaluated on both real-world and simulation DCs datasets, and SGPINN all achieved the best performance, demonstrating the generalization of SGPINN. Compared with APINN, SGPINN reduces MAE and RMSE by 3.57% and 3.58%, respectively, in real-world case. The experimental result s indicate that graph physical

representation provides clear advantages over baseline models. The learned equivalent thermal capacitance and heat flow terms provide a qualitative reference to guide the thermal management of DCs. In the future, adaptive topology or workload heat generation can be further incorporate to as learning factors to improve model generalization.

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