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Rapid prediction of structural thermo-mechanical responses based on graph neural network

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Abstract: Fire is one of the most serious hazards that structures could suffer during their service lives, which would impose devastating losses on lives and properties. Rapid prediction of thermal behavior and structural responses is essential for the assessment of structural fire safety. However, finite element methods (FEMs) typically come with high computational costs, and thus fail to meet the demand for fast computation. This study proposes a graph neural network (GNN)-based framework to predict structural thermo-mechanical responses. The geometric and physical information, e.g., fire area and boundary condition, is considered in the vertex embedding. Taking the fire position and heat flux as input, the proposed GNN model is able to provide temporal prediction on temperature, stress and displacement simultaneously. A physics-informed aggregate function is introduced in the message passing phase, enabling the heat conduction to be well captured by the message passing process. Moreover, new prediction schemes have been proposed to eliminate the effect of error accumulation in the rollout prediction. Two numerical examples are employed to verify the effectiveness of the proposed GNN-based framework. The results show that the proposed prediction model accurately predicts structural thermo-mechanical responses even for large-scale complex structures using a small number of training data, and runs an order of magnitude speedup compared to the FEM. The proposed GNN-based framework is of great potential for the application of real-time response prediction of large-scale realistic structures during fire emergencies.

Keywords: structural fire safety; real-time prediction; graph neural network; heat transfer; thermo- mechanical



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1. Introduction

Fire is one of the most serious hazards that buildings and infrastructures could suffer during their service lives [1]. For buildings, the fire-induced failure of structural components will trap large numbers of people inside the building, and thus leads to devastating losses of lives and properties [2,3]. Compared with building fires, bridge fire incidents typically caused by traffic accidents of vehicles are much more severe, as the resulting gasoline fires have a fast heating rate and a higher peak temperature [4]. Previous studies reveal that more than 3% of bridge failures are caused by fires, which are higher than those resulted from earthquake and winds [5]. Therefore, research on the structural performance during fire emergencies is of great significance for guiding the rescuing actions, ensuring structural safety and improving structural resilience [6].

Existing approaches for structural fire analysis are mainly categorized into two major groups, *i.e.*, experimental methods and numerical analysis. Alos-Moya *et al.* [7] conducted open air fire tests of a composite bridge to investigate the structural responses to 4 fire scenarios. Wickström *et al.* [8] carried out an indoor fire test on a beam for predicting heat transfer using the adiabatic surface temperature. However, experimental tests are costly to carry out and usually cannot reproduce some important fire characteristics [9]. In regard to numerical methods, the computational fluid dynamics (CFD) is a commonly used technique for calculating the heat release rate (HRR) and adiabatic surface temperature of structures [10]. Some researchers combined the CFD with finite element methods (FEMs) to simulate fire dynamics, thermal behavior and structural responses [11]. The fire simulation is first carried out using the CFD, and then the temperature results as the predefined field is transferred into the FE model for the sequentially coupled thermo-mechanical analysis [4,9,12–14]. For simplicity purposes, standard fire curves are employed as the thermal boundary condition instead of conducting CFD fire simulation [15,16]. Moreover, in addition to the adiabatic surface temperature acting as the convection boundary, the heat flux is another commonly used thermal load [17]. However, the numerical methods for structural fire analysis are time-consuming and unable to provide real-time structural responses during fire emergencies.

Machine learning (ML) have been increasingly popular in structural engineering problems [18], and provides alternative approaches for the prediction of structural fire responses. Dung *et al.* [19] used the multiple linear regression and random forest to predict the temperature distribution along the thickness direction of a steel slab. These simple machine learning models also can be applied for predicting complete temperature profiles of 3D structural members [20]. Since the temperature spot in a 2D thermogram is similar to the pixel of an image, many researchers employed convolutional neural networks (CNNs) for fast prediction of thermal distribution [21]. Edges [22–24] or surface [25] where the thermal load is applied are assigned with different grey values from other pixels on the input image, and the output of CNN is the temperature cloud diagram. For 3D heat conduction, Wang *et al.* [26] employed the U-net to predict the temperature field of a solid cube. Moreover, CNNs have been applied to forecast spatial and temporal temperature distribution of urban and tunnel fires [27–29]. In terms of thermo-mechanical analysis, Ye *et al.* [30] developed an FE-based

ML framework to predict the structural displacement of a steel frame based on temperature data. Later, they applied the proposed method for real-time prediction of the displacement and stress of a roof structure under indoor fire [31]. Although the aforementioned approaches have shown excellent accuracy and efficiency in predicting structural fire responses, they generally perform prediction from the input state to the output state as “black box” models, which do not account for the principled physical laws governing the structural system. Moreover, when dealing with complex large-scale structures or irregular FE meshes, CNNs and other conventional ML methods rely heavily on complicated network architectures, which requires large volume of training data to guarantee the robustness and convergence.

Recently, as another group of ML approaches, graph neural networks (GNNs) have demonstrated a great potential in various scientific fields, such as social network analysis [32,33], drug development [34,35] and traffic forecasting [36,37]. Since the message-passing mechanism is employed to capture complex relationships and features between nodes and edges, GNNs are capable of generalizing to systems with varying sizes and structures [38,39]. Moreover, unlike CNNs, which are restricted to Euclidean data, GNNs are well suited to deal with mesh-based and particle-based non-Euclidean data structure [40]. GNNs have been successfully applied to predict structural stress distribution [41], deformation [42] and dynamic responses [43] to accelerate numerical simulation of FE. However, the existing GNN-based algorithms are typically data-driven models, which neglect distinctive physical laws and mechanical principles for structural analysis. Furthermore, these approaches are mainly employed for dealing with simple structures, such as beam and frame models, but seldom applied to large-scale complex structural analysis.

In this study, a GNN-based framework is proposed to predict the thermal behavior and structural responses under fire hazard. The physical information is considered in the encoder-processor-decoder architecture of the proposed GNN, which enables the temperature to be predicted accurately through the aggregation in the graph convolution. Moreover, two new prediction schemes have been proposed to eliminate the effect of error accumulation in the rollout prediction on the temperature. For the thermal stress and displacement prediction, a new vertex embedding method is developed, in which the surface heat flux instead of the predicted temperature is embedded in the thermal attribute. Consequently, unlike the conventional FEMs based on the sequentially coupled thermo-mechanical analysis, the proposed GNN model is able to predict the structural thermo-mechanical responses simultaneously.

2. Methodology

2.1. GNN model

The data structure of a graph can be expressed as $G=(V,E)$, where V is a set of objects called vertices and E is a set of links between paired vertices called edges. To describe the adjacency relation for graph representation, an adjacency matrix A is proposed:

$$A_{ij} = \begin{cases} 1, & \text{if } \{v_i, v_j\} \in E \text{ and } i \neq j, \\ 0, & \text{otherwise,} \end{cases} \quad (1)$$

where $\{v_i, v_j\} \in E$ denotes two vertices v_i and v_j are connected by a link in E .

According to the numerical simulation results, the thermal and mechanical responses of some nodes in the FE model almost remain unchanged throughout the fire duration, and thus it is inefficient to encode these nodes into the graph representation. In this regard, only those nodes whose fire responses are beyond a certain threshold will be considered as the prediction area. The nodes and edges in the FE mesh within the prediction area are embedded as V and E in the graph data structure, respectively.

2.1.1 Graph embedding

The information of the FE model should be encoded into the graph structure for numerical simulation. In this study, the vertex attribute h_{v_i} for each vertex $v_i \in V$ is defined as

$$h_{v_i}^T = h_{v_i}^{posT} \oplus h_{v_i}^{bcT} \oplus h_{v_i}^{heat}, \quad (2)$$

$$h_{v_i}^M = h_{v_i}^{posM} \oplus h_{v_i}^{bcM} \oplus h_{v_i}^{heat} \oplus h_{v_i}^{init} \oplus h_{v_i}^f, \quad (3)$$

where the superscripts T and M represent the attribute used for the prediction of thermal and mechanical responses, respectively, and $\oplus$ indicates the concatenation operation. Normally, the geometric boundary in the heat transfer is the edge or interface of the structure, while flexible or rigid supports work as the mechanical boundary. $h_{v_i}^{pos}$ encodes the position of the target node, and consists of the distance to the centroid of the fire area and the distance to the nearest boundary. For some complex structures, geometric boundaries are different for thermal and mechanical predictions. Therefore, $h_{v_i}^{posT}$ and $h_{v_i}^{posM}$ are used in Equations (2) and (3) to distinguish $h_{v_i}^{pos}$ embedded in $h_{v_i}^T$ and $h_{v_i}^M$. As illustrated in Figure 1, taking the 2D slab as an example, the geometric vertex attribute $h_{v_i}^{posT} = h_{v_i}^{posM} = (x_{fire-center}, y_{fire-center}, x_{boundary}, y_{boundary})$. To furtherly consider the influence of boundary conditions, one-hot encoding is employed in $h_{v_i}^{bc}$ to distinguish the boundary conditions of each node in the mesh element. $h_{v_i}^{bcT}$ and $h_{v_i}^{bcM}$ denote the thermal and mechanical boundary conditions, respectively. Moreover, nodes which are heated should contain the heat flux $q_{surface}$ in the thermal attribute $h_{v_i}^{heat}$. In terms of mechanical response prediction, more attributes should be considered as shown in Equation (3), where the initial stress and displacement field under gravity are included in $h_{v_i}^{init}$ and $h_{v_i}^f$ encodes the magnitude of the external load.

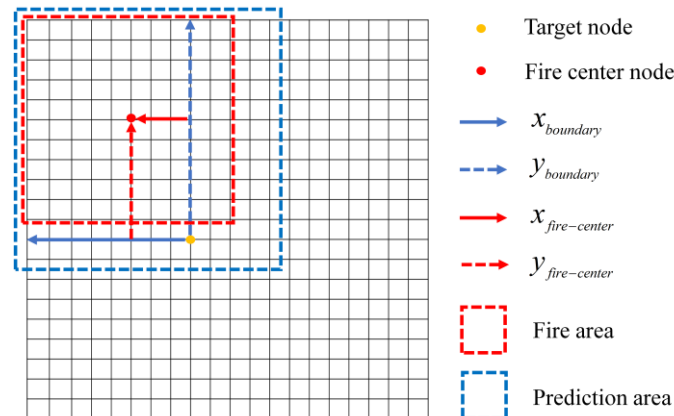


Figure 1. Geometric vertex attribute of a 2D slab.

The global attribute vector θ contains properties shared by all vertices in the graph, *i.e.*, time and material parameters. To reduce the complexity level of the model and address the over-smoothing problem [41], the global attribute vector θ is directly concatenated into the vertex embedding $\mathbf{h}_{v_i}$ as

$$\hat{\mathbf{h}}_{v_i} = \mathbf{h}_{v_i} \oplus \theta. \quad (4)$$

2.1.2 Encoder-Processor-Decoder architecture

Encoder. The encoder embeds each vertex attribute vector $\hat{\mathbf{h}}_{v_i}$ into a higher dimensional space according to

$$\mathbf{h}_{v_i}^0 = f_{en}(\hat{\mathbf{h}}_{v_i}), \quad (5)$$

where the embedding function f_{en} is the three-layer MLP in this study, and $\mathbf{h}_{v_i}^0$ is the input of the first layer in the GNN processor.

Processor. The processor updates the latent graph through $k=1, 2, \dots, K$ message passing steps. Unlike basic graph convolution network (GCN) which only considers the adjacency relationship during message passing [44], this study uses a method similar to SAGEConv [45] which enables a vertex to aggregate feature information from its neighbors. In the k th layer of the processor, the hidden representation $\mathbf{h}_{v_i}^{k-1}$ of each vertex is updated according to

$$\mathbf{h}_{N(v_i)}^k = \text{AGGREGATE}\left(\left\{\mathbf{h}_{v_j}^{k-1}, \forall v_j \in N(v_i)\right\}\right), \quad (6)$$

$$\mathbf{h}_{v_i}^k = \phi\left(\mathbf{W}^k \cdot \left(\mathbf{h}_{v_i}^{k-1} \oplus \mathbf{h}_{N(v_i)}^k\right)\right), \quad (7)$$

where $N(v_i)$ denotes the neighbor nodes of v_i , AGGREGATE is the aggregator, $\mathbf{W}^k$ is a learnable weight matrix, and $\text{ReLU}(\cdot)$ is employed as the nonlinear activation function ϕ .

Decoder. The decoding stage makes the prediction from the final latent graph. For each vertex $v_i \in \mathbf{V}$, the structural fire responses, *i.e.*, T_i , σ_i and u_i , are extracted as

$$\hat{y}_i = f_{de}(\mathbf{h}_{v_i}^K), \quad (8)$$

where f_{de} is also implemented using three-layer MLP.

In order to train the proposed GNN model through back propagation, mean square error (MSE) is chosen as the loss function

$$Loss_{\text{MSE}} = \frac{1}{n} \cdot \sum_{i=1}^n (y_i - \hat{y}_i)^2, \quad (9)$$

where y_i is the structural fire response calculated by the FE solver, and n is the number of vertices in a graph. The overall architecture of the proposed GNN model is shown in Figure 2.

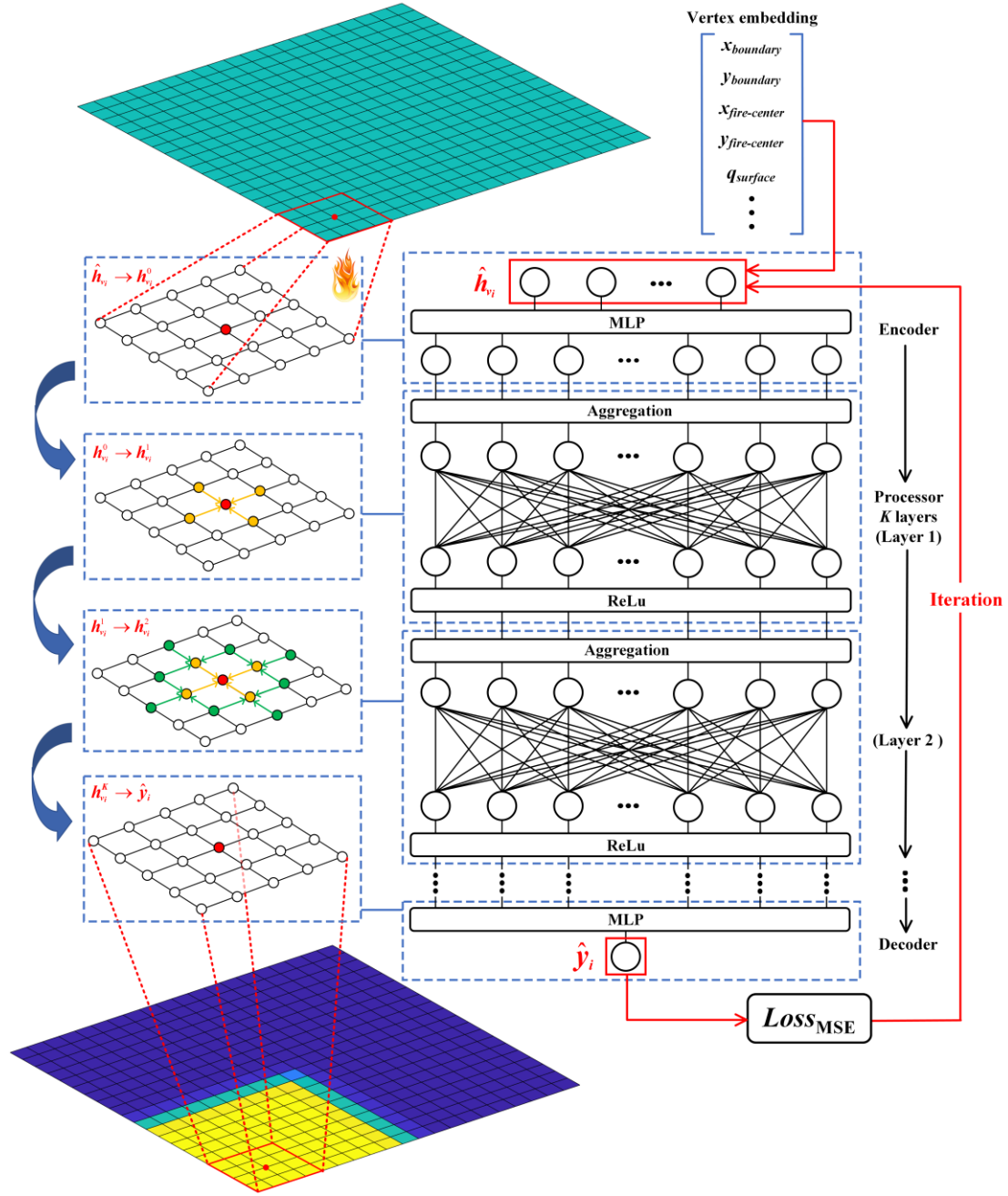


Figure 2. GNN architecture.

2.1.3 Heat conduction and its relation with message passing in GNN

The 2D transient heat conduction formula can be expressed as the following partial differential equation

$$\frac{\partial T}{\partial t} = a \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + \frac{q_v}{\rho c}, \quad (10)$$

where $a = \lambda / (c\rho)$, λ is the thermal conductivity, c represents the heat capacity, and ρ denotes the material density. q_v is the body heat flux applied to the area. However, it is computational intractable to derive an analytical solution of Equation (10) to obtain the spatial and temporal distribution of the temperature T . To this end, Taer and Duda [46]

proposed a numerical method to solve the transient heat conduction problem, in which the heat conduction equation was modified to an approximate discretized form. As shown in Figure 3, for the node v_i with four neighbors, the Equation (10) can thus be rewritten as

$$\frac{T_i^{k+1}}{\Delta t} - \frac{q_v}{\rho c} = a \left[\frac{T_{j_1}^k}{(\Delta x)^2} + \frac{T_{j_2}^k}{(\Delta x)^2} + \frac{T_{j_3}^k}{(\Delta y)^2} + \frac{T_{j_4}^k}{(\Delta y)^2} \right] + \left(\frac{1}{\Delta t} - \frac{2a}{(\Delta x)^2} - \frac{2a}{(\Delta y)^2} \right) T_i^k, \quad (11)$$

where Δx and Δy are the length and width of the discrete mesh, and Δt is the time interval. The superscript represents the time step and subscript denotes the node number. In terms of uniform mesh, *i.e.*, $\Delta x = \Delta y$, the Equation (11) is further simplified as:

$$\frac{\Delta x^2}{\Delta t} T_i^{k+1} - \frac{\Delta x^2}{\rho c} q_v = a(T_{j_1}^k + T_{j_2}^k + T_{j_3}^k + T_{j_4}^k) + \left(\frac{\Delta x^2}{\Delta t} - 4a \right) T_i^k. \quad (12)$$

The left hand of the heat conduction equation contains the temperature of node v_i at $(k+1)$ th time step, while the aggregation of temperatures of 4 neighboring nodes and the targeted node temperature at k th time step are on the right side.

Inspired by the expression of the heat conduction, the mean function is employed as the aggregator in the message passing phase in this study. Consequently, according to Equations (6) and (7), the local message passing formula for the vertex v_i can be rewritten as:

$$\mathbf{h}_{v_i}^{k+1} = \phi \left(\mathbf{W}^k \cdot \left(\frac{1}{4} (\mathbf{h}_{v_{j_1}}^k + \mathbf{h}_{v_{j_2}}^k + \mathbf{h}_{v_{j_3}}^k + \mathbf{h}_{v_{j_4}}^k) \oplus \mathbf{h}_{v_i}^k \right) \right), \quad (13)$$

$\mathbf{h}_{v_i}^k$ of each vertex in the graph is updated to $\mathbf{h}_{v_i}^{k+1}$ through concatenating the vertex attribute with the aggregation of all its neighboring node attributes. It can be found that Equations (11), (12) and (13) all have a similar expression if $\mathbf{h}$ is viewed as $\mathbf{T}$. The message passing in GNN perfectly matches the heat conduction in this study. The temperature of the target node can be predicted accurately using the messages from its adjacent nodes, since the heat conduction has been well captured by the message passing process. The effectiveness of the aggregation Equation (13) will be verified in Subsection 3.2.2.

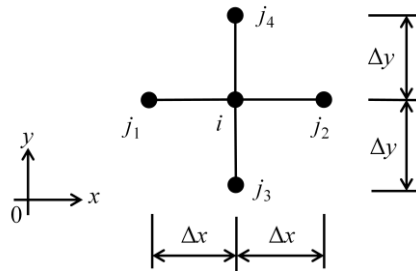


Figure 3. Diagram of nodes that lie inside the analyzed region of heat conduction.

2.2. Thermo-mechanical prediction

2.2.1 Temperature prediction

In the graph network-based simulators (GNS) proposed by Sanchez-Gonzalez *et al.* [38], the temporal data in complex physical systems is predicted by a multi-step rolling prediction mode. As shown in Figure 4 (left), the GNS model is composed of K GNN-based single-step predictors. At the first step, only the initial features are used as the input to predict the temperature T^1 , which is then concatenated into the thermal feature $\mathbf{h}_{v_i}^{heat}$ before being fed into GNN₂. For this rollout prediction scheme, the GNN prediction from the previous step is used as the input of the current step. Consequently, the error may accumulate to a large extent as the number of the time step increases.

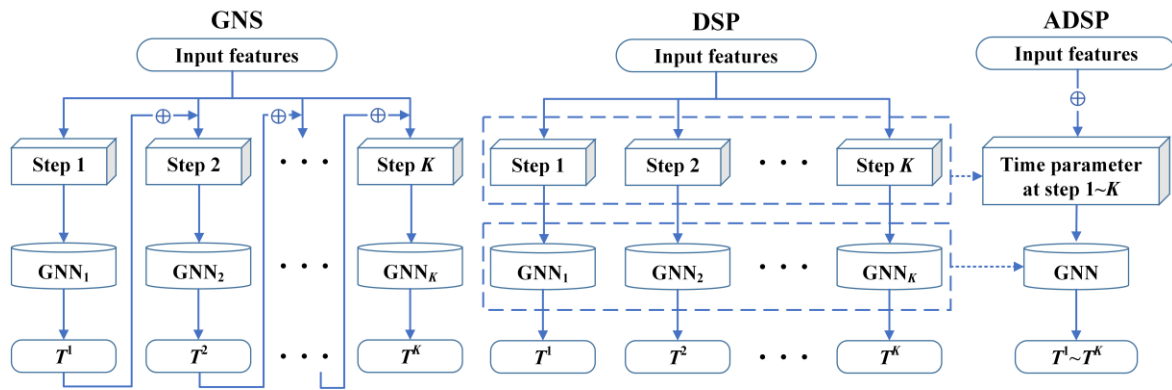


Figure 4. Flowchart of GNS (Adapted from [38]), DSP and ADSP.

To overcome the error accumulation, a designated-step prediction (DSP) scheme is proposed in this study, in which the temperature $T^{(k-1)}$ obtained from the $(k-1)$ th step is no longer considered in the thermal feature for predicting T^k at the k th step. The flowchart of the DSP is shown in the middle of Figure 4. However, since the input of DSP lacks the temperature results predicted previously, the prediction accuracy may be slightly lower than that of GNS.

Since it is computationally expensive to train one GNN for every time step in practical applications, an advanced DSP (ADSP) method is also proposed in this study, in which GNNs aimed at different designated moments in DSP are combined into a single one without splitting the training set. As introduced previously, the time parameter is embedded into the global feature θ in the proposed ADSP framework. The accuracy and efficiency of GNS, DSP and ADSP will be compared in Subsection 3.2.2 to verify the effectiveness of the proposed method.

2.2.2 Thermal stress and displacement prediction

In sequentially coupled thermal-mechanical analysis, the temperature results T^k from the thermal analysis serve as the input predefined field for mechanical analysis at the k th step, as shown in Figure 5. When using the GNN to predict mechanical responses, it is

straightforward to embed thermal information in the vertex attribute $\mathbf{h}_{v_i}$. Previous studies embed the predicted node temperature T_i in the thermal attribute $\mathbf{h}_{v_i}^{heat}$ to form the local embedding $\mathbf{h}_{v_i}^M$ in GNN for mechanical prediction [30], which is denoted as Plan A as shown in Figure 5.

As introduced in Subsection 2.2.1, error exists in the predicted temperature, which would lead to accumulated error for the subsequent prediction of mechanical responses. In this regard, a new embedding method called Plan B is proposed to eliminate the effect of error accumulation. The surface heat flux $q_{surface}$ instead of the predicted node temperature $T_{v_i}^k$ is embedded in the thermal attribute $\mathbf{h}_{v_i}^{heat}$, and the fire duration at the targeted step is set as the global feature θ in this study. Moreover, the proposed Plan B skips the prediction step of heat conduction and forecast stress and displacement directly, which further increases the efficiency of the proposed algorithm. Figure 5 compares the Plan A and Plan B in terms of the forecasting procedure and embedded features. Results of the two prediction plans will be compared in Subsection 3.3.

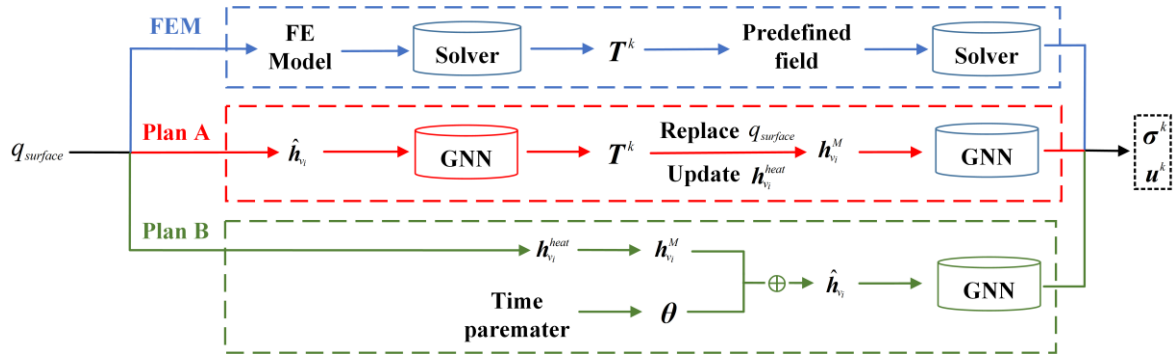


Figure 5. Comparison between FEM, Plan A (Adapted from [30]) and Plan B in prediction of mechanical responses.

3. Numerical example 1: a steel slab

3.1. FE modeling

In this study, ABAQUS is employed as the FE solver to simulate structural fire responses [47]. The first example is a simply supported steel slab with the size of 2 m $\times$ 2 m. Given that the thickness is only 10 mm, the slab is modeled using 4-node shell elements with a size of 100 mm $\times$ 100 mm, resulting in 400 elements and 441 nodes in total as shown in Figure 6. The steel grade is Q235, of which the material properties are determined according to Eurocode (EC) 3 [48], including the expansion ratio α , specific heat capacity c and thermal conductance k . The degradation of the steel's yield strength and Young's modulus during the heating process is also considered in this study.

Different fire scenarios are simulated through varying fire positions and heat fluxes. The slab is equally divided into 4 parts, and only one of them is heated with the surface heat flux ranging from 25 kW/m² to 65 kW/m². The room temperature is set to 0 °C. To verify the inductive ability of the proposed GNN prediction model, the training set only contains 122

fire scenarios. For temporal prediction of heat conduction, the node temperatures are extracted from ABAQUS every 1 min for one fire scenario. The fire duration is 10 min, and thus 10 pieces of temperature data are submitted for mechanical analysis to simulate Von Mises Stress and node displacement at 10 time steps. Consequently, there are totally $122 \times 10 = 1220$ training samples for prediction of the slab's fire responses.

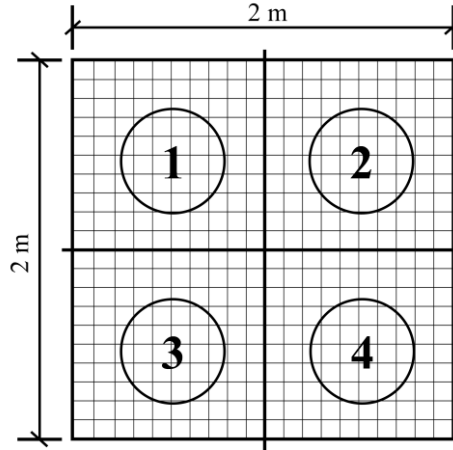


Figure 6. Division of the steel slab.

3.2. Prediction results of temperature

3.2.1 Comparison of temporal prediction methods

Three prediction schemes, *i.e.*, GNS, DSP and ADSP, are compared with a learning rate of 0.0001 for around 2000 iterations. Early stopping is introduced to avoid overfitting. Mean absolute error (MAE), mean absolute percentage error (MAPE) and MSE are used to evaluate the accuracy of the GNN model. MAE and MAPE are formulated as:

$$Loss_{MAE} = \frac{1}{n} \cdot \sum_{i=1}^n |y_i - \hat{y}_i|, \quad (14)$$

$$Loss_{MAPE} = \frac{1}{n} \cdot \sum_{i=1}^n \left| \frac{y_i - \hat{y}_i}{y_i + \varepsilon} \right| \times 100\%, \quad (15)$$

where ε is typically set as a small value to avoid computation error when the ground truth temperature is 0.

Figure 7 illustrates the MSEs of 10 testing samples for GNS, DSP and ADSP. MSEs of three different prediction schemes do not show much difference at the beginning 3 time steps, while the MSE of GNS rises dramatically since the 4th time step due to the accumulated error. MSEs of DSP and ADSP increase steadily with the increase of the time step, while are still below 10 at the 10th time step, indicating that the proposed DSP and ADSP is effective in eliminating error accumulation.

The FE computational process is conducted on a PC with an Intel®i7-8700™CPU (8 cores, 2.5 GHz) and 32 GB of RAM. As shown in Table 1, the runtime using ABAQUS is compared with that in three prediction models. The GNN models achieve almost 20 times

speedup compared with the FEM. Given that DSP and ADSP have the same number of training epochs, the training times of DSP and ADSP are 18,637.12 s and 16,361.39 s, respectively. Although both DSP and ADSP are able to achieve precise and quick prediction, ADSP outperforms DSP in terms of computational efficiency of model training. Figure 8 displays the absolute error distribution of ADSP. It is found that ADSP could accurately predict the descending gradient from high-temperature region to low-temperature region.

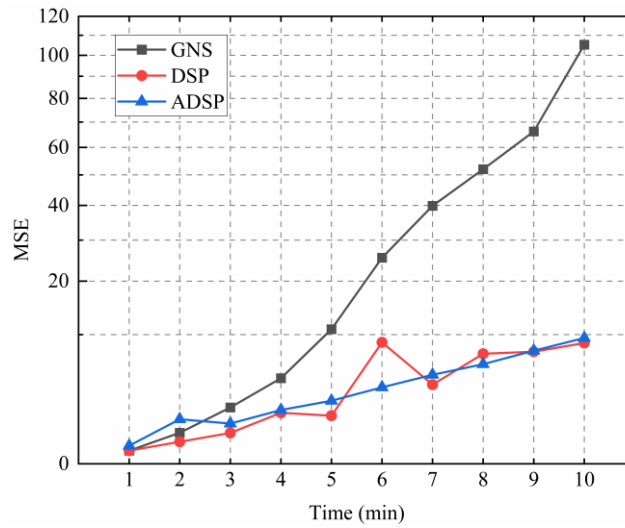


Figure 7. MSEs of the testing set at 10 time steps.

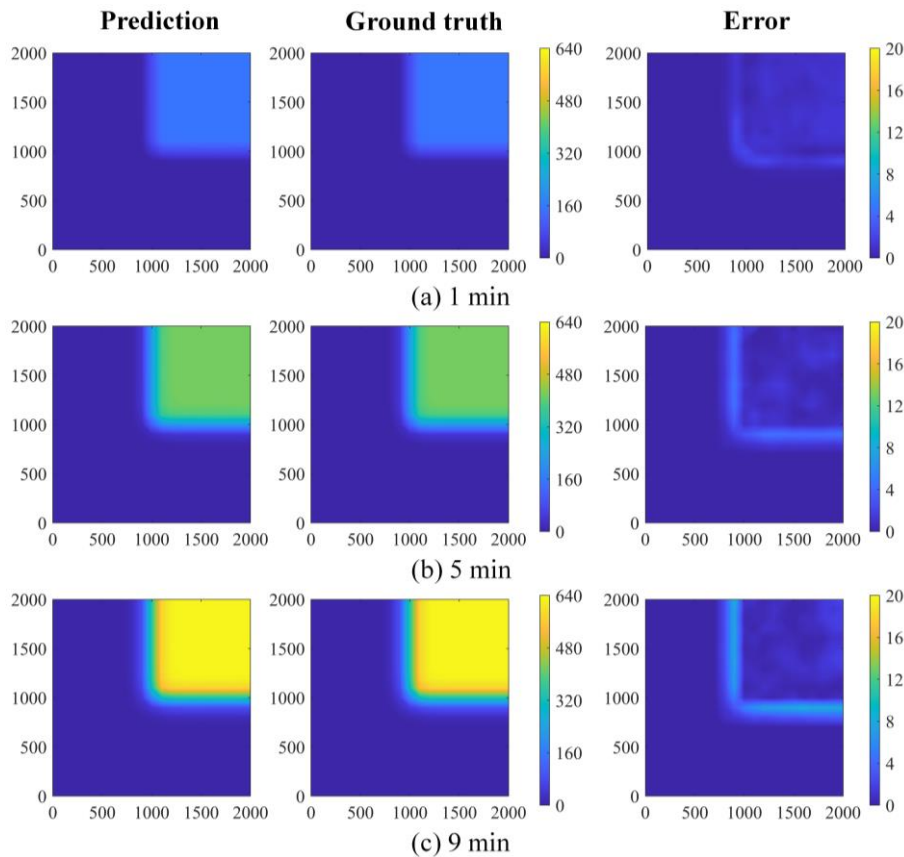


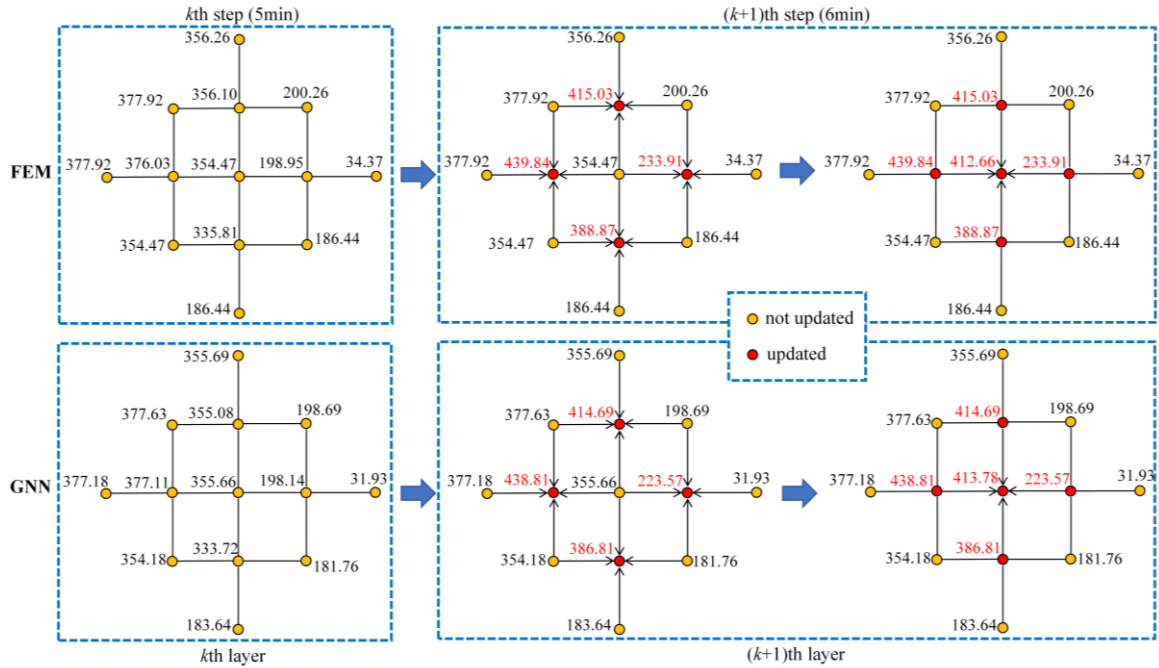
Figure 8. Error distribution in temperature prediction (length unit: mm, temperature unit: °C).

Table 1. Runtimes comparison in heat transfer calculation.

Method	Time (s)	Speedup
FEM	88.85	-
GNS	4.44	20.01
DSP	4.37	20.33
ADSP	4.99	17.81

3.2.2 The effect of physics-informed aggregation function

To illustrate the relation between the heat conduction and message passing in GNN as introduced in Subsection 2.1.3, Figure 9 compares the updating process of a randomly selected node in FEM and GNN. The yellow circle represents the node temperature at the k th step, while the red circle means its information has been updated to $(k+1)$ th step. As shown in Figure 9, the heat conduction uses current temperatures of adjacent nodes to calculate temperature of the target node in the next time step. In GNN, 4 adjacent nodes of the target node would first receive hidden representations of their neighbors in the k th layer before updating information of the target node to the $(k+1)$ th layer. It could be found that GNN's message passing and aggregation perfectly matches the FEM updating between two adjacent time steps.

**Figure 9.** Process of node updating in FEM and GNN (unit: °C).

To further demonstrate the effectiveness of the aggregation method through adjacency relationship, a new variable R_{Heat} is introduced to represent the physical residual generated by GNN, which is calculated by:

$$R_{Heat} = \left(\left(\frac{\Delta x^2}{\Delta t} T_i^{k+1} - \frac{\Delta x^2}{\rho c} q_v \right) - \left(a(T_{j_1}^k + T_{j_2}^k + T_{j_3}^k + T_{j_4}^k) + \left(\frac{\Delta x^2}{\Delta t} - 4a \right) T_i^k \right) \right). \quad (16)$$

R_{Heat} of all nodes shown in Figure 9 is no more than 1.5×10^{-4} and the discrepancy between two sides of the heat balance equation is only around 2%.

3.3. Prediction results of thermal stress and displacement

Since the vertical displacement is much larger than that on the other two orthogonal directions, only the vertical node displacement is considered in this study. For the slab structure, the mechanical boundary condition is the same as the thermal boundary condition, and thus $\mathbf{h}_{v_i}^{bCM} = \mathbf{h}_{v_i}^{bCT}$ in this case. The gravity and other external forces are neglected in this case, and $\mathbf{h}_{v_i}^M$ thus does not contain $\mathbf{h}_{v_i}^{init}$ and $\mathbf{h}_{v_i}^f$.

MAPEs of stress and displacement predicted by Plan A and Plan B are compared in Figure 10. As introduced previously, the error in the predicted temperature for Plan A would lead to error accumulation for the mechanical responses. To illustrate the effect of the accumulated error, MAPE of Plan A using the true temperature is also compared here. In terms of stress prediction, Plan A has a higher mean error and median level than Plan B even using the true temperature embedding. Moreover, there is only 1 abnormal testing sample with error above 10% in Plan B, while the number rises to 7 in Plan A using predicted temperature. For displacement prediction, the mean level of MAPEs of Plan A with and without accumulated error reaches 16.7% and 13.1%, respectively, which do not achieve satisfactory accuracy. The mean error of Plan B is only 4.29%, and approximately 75% of the testing samples reach an accuracy beyond 95% except for 1 outlier with the error above 10%. Overall, the prediction error for displacement is greater than that for stress. Even if the true temperatures are employed to predict mechanical responses, the prediction accuracy of Plan A is still lower than that of Plan B, which demonstrates the superiority of the proposed embedding method.

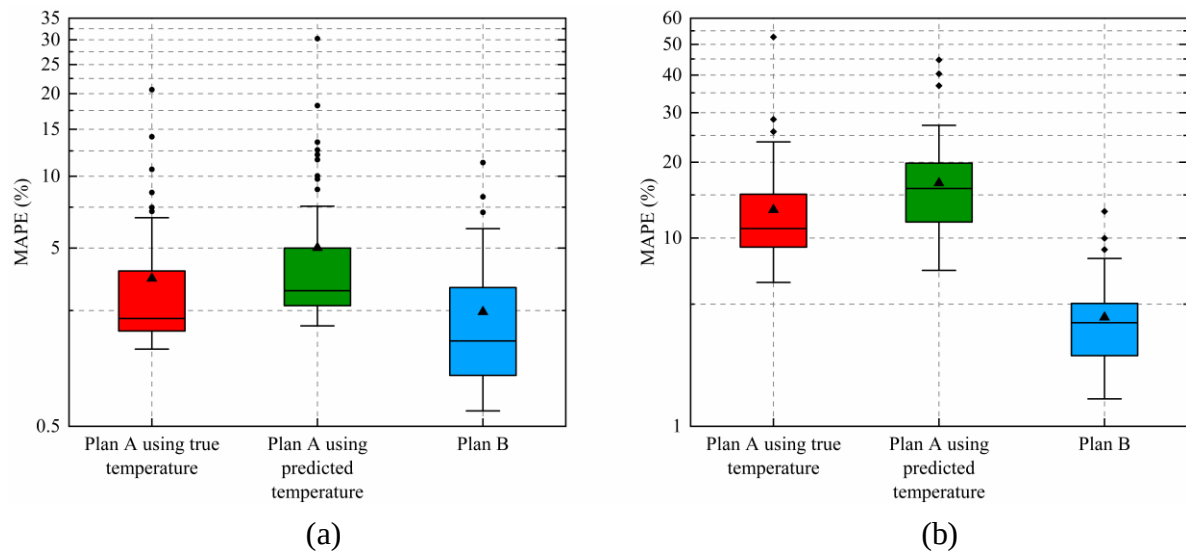


Figure 10. Box plots of MAPE of Plan A and Plan B, where the dots indicate the outlier points, the triangles represent the mean errors and black lines in boxes represent the median errors: (a) stress, (b) displacement.

The runtimes for stress and displacement prediction are compared in Table 2. If time consumed for temperature prediction is taken into account, it takes 9.03 s for Plan A to predict stress and displacement of one fire scenario with 10 time steps, which is 5.62 s lower than Plan B. However, either method is much faster than ABAQUS, which takes 24.29 s for one single time step. As shown in Table 2, Plan B achieves more than 70 times speedup compared with the FEM. If the time consumed in the heat transfer calculation is considered, it takes the FE solver 331.75 s to get mechanical results, and the speedup ratio of Plan B will increase to 97.29. Therefore, Plan B is more efficient and accurate for prediction of mechanical responses, and thus will be employed in the following case study.

Table 2. Runtimes comparison in thermal stress and displacement prediction.

Method	Time (s)	Speedup
FEM	$24.29 \times 10 = 242.9$	-
Plan A	9.03	26.90
Plan B	3.41	71.23

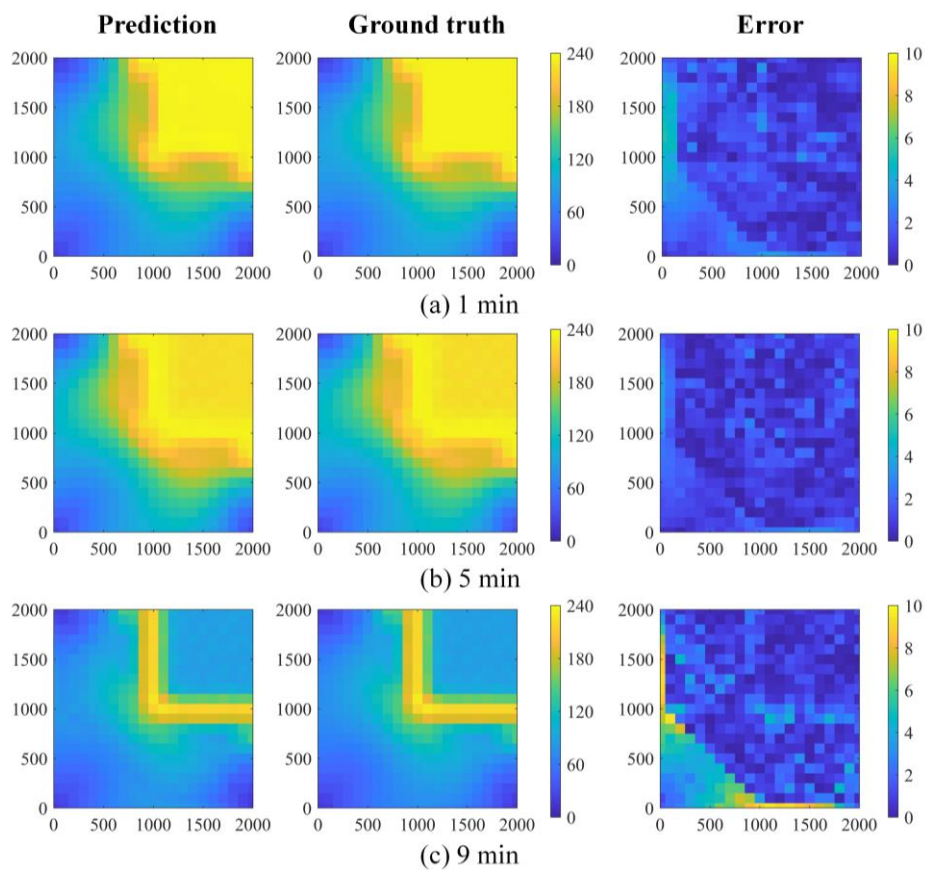


Figure 11. Error distribution in stress prediction (length unit: mm, stress unit: MPa).

To investigate whether the proposed GNN model could enable accurate prediction of complicated mechanical responses in the heated area, the error distributions of stress and displacement are presented in Figure 11 and Figure 12, respectively. The thermal stress in the yield part of the steel slab will decrease in the last few minutes due to the strength

degradation, and the GNN model achieves accurate prediction for the changing stress of these yield nodes. As shown in Figure 12, heated nodes move upward at the beginning due to the thermal expansion, and then large deflection occurs around the fire center because of the strength degradation. According to the error distributions in Figure 12, the upward and downward moving trends of yield nodes have been learned by the GNN model, and the absolute error in displacement prediction is controlled to a relatively low level.

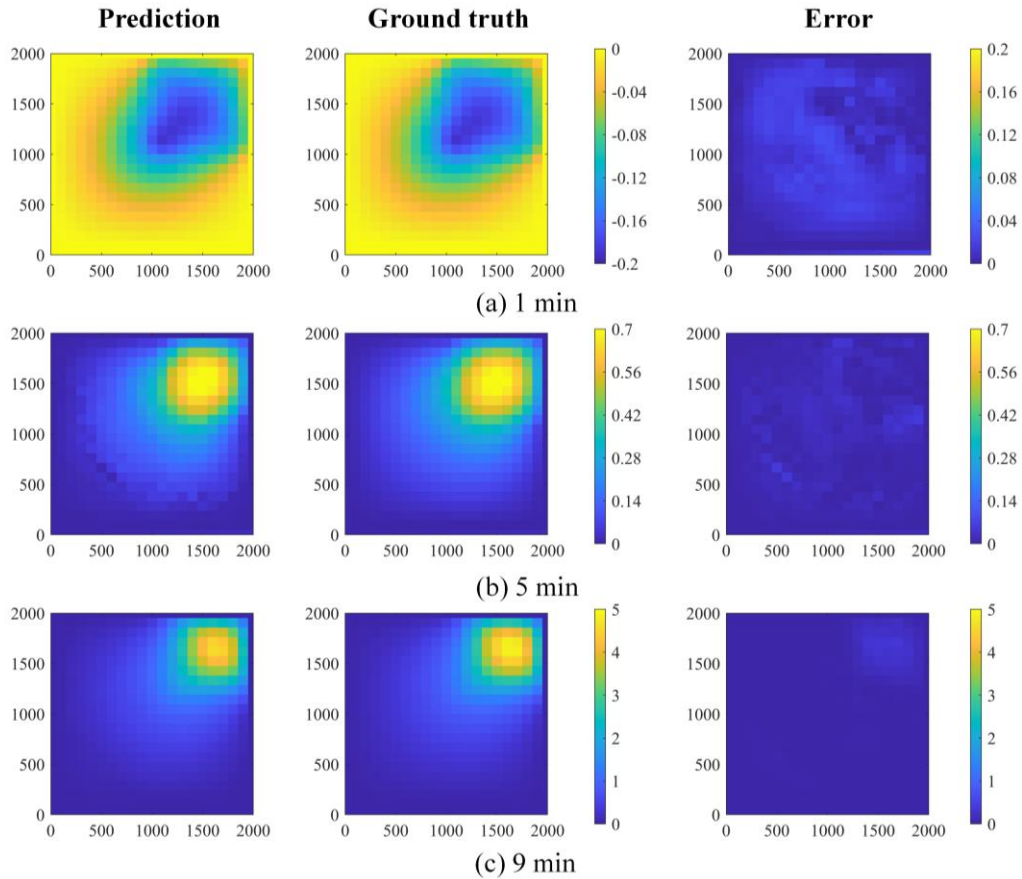


Figure 12. Error distribution in displacement prediction, where downward displacement is positive (unit: mm).

4. Numerical example 2: a cable-stayed bridge

4.1. FE modeling

A cable-stayed bridge is numerically analyzed to illustrate the proposed GNN model for rapid structural thermo-mechanical response prediction, as shown in Figure 13. The bridge is of length 392 m, and has 64 cables with the diameter of 120 mm. The cross section of the girder is shown in Figure 14, and the steel grade is Q345. The thickness of the top flange, bottom flange and web plates in the girder is 40 mm. For the sake of simplicity in the dataset generation, a simplified method of FE modeling is employed here. The girder is simply supported, and is discretized into 4-node shell elements with a size of $1.625 \text{ m} \times 4 \text{ m}$. The beam element with the size of 5 m is assigned to the cable. Consequently, there are 1584 and

1000 nodes in the girder and cables, respectively. Concrete piers and pylons are not assembled into the FE model due to their excellent resistance to the fire hazard, and instead their constraint effect is considered as simple supports for the girder and cables. The material properties of the cable are obtained from Lee *et al.* [17], where the Young's modulus is 188 GPa and yield strength is 1570 MPa at room temperature.

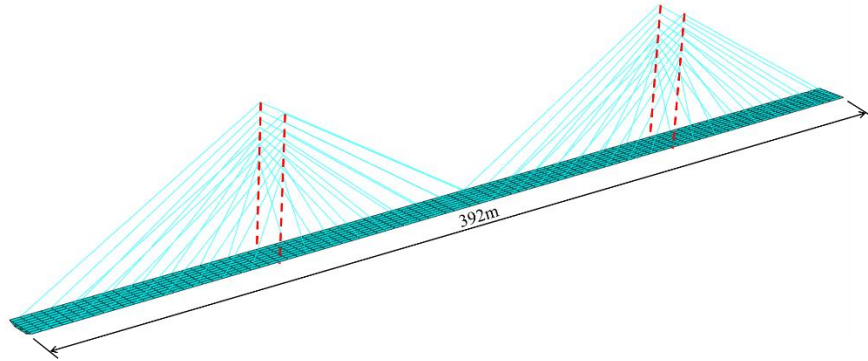


Figure 13. FE model of the cable-stayed bridge.

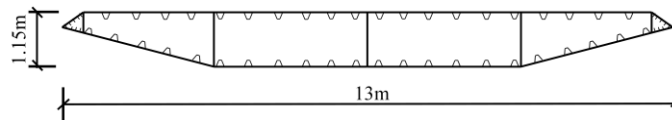


Figure 14. Cross section of the girder.

The bridge fire caused by the tanker accident is considered in this case. The heat flux transmitted from the fire zone can be calculated using the radiation model for open-air pool fires [49]. According to Lee *et al.* [17], the effect of the tanker fire is limited in a cube with a height of 15 m. To form the fire zone, the deck is divided into 128 sections each with a width of 3.25 m and a length of 12 m according to the size of the tanker. As shown in Figure 15, if the accident happens on the left or right side of the bridge, the cables will be affected by fire as well.

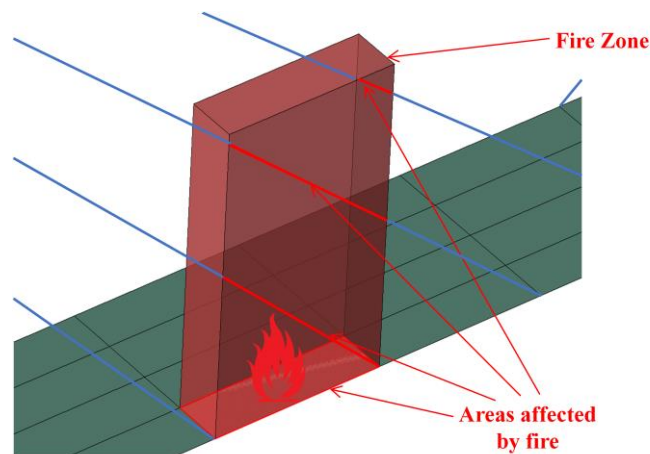


Figure 15. Areas in girder and cables affected by fire.

Different fire scenarios are created by varying the fire area and heat flux. The surface heat flux for each fire scenario is randomly selected from the range between 30 kW/m² and 60 kW/m², and the rise and descent phases of the heat flux curve are not considered for simplicity. To apply the thermal load to cables, the surface heat flux should be converted into the body heat flux. Before applying the temperature field for mechanical analysis, the displacement and stress caused by the gravity of the girder and accident vehicle are calculated in advance. The car load varying from 20 t to 30 t is imposed on the same discretized part of the girder where the thermal load is applied. In this case, the entire dataset contains 202 fire scenarios, and 10 of those are randomly selected as the testing set. The fire duration is set as 30 min for each fire scenario. Structural responses are simulated in ABAQUS every 1 min, and thus there are $192 \times 30 = 5760$ pieces of training data.

4.2. Prediction of temperature

As introduced in Subsection 3.2.1, the proposed temporal prediction method ADSP is adopted here. Most features in $\mathbf{h}_{v_i}^T$ are same as those in the slab case. For the bridge structure, the geometric boundary of girder for the heat conduction only involves its left and right edges, and thus $(x_{boundary}, y_{boundary})$ in $\mathbf{h}_{v_i}^{post}$ in this case is the distance to the nearest edge of the bridge.

There are 3 kinds of nodes with special boundary conditions, including:

- (1) nodes connected with heated cables;
- (2) nodes connected with unheated cables;
- (3) nodes connecting the flange and web.

To distinguish these nodes with others, $\mathbf{h}_{v_i}^{bct}$ should be converted into one-hot code with a dimension of 4.

Although the bridge girder is not a simple 2D slab structure due to the cables and web plates below the deck, MAPEs of the prediction results are still at a low level of below 1.5% at all time steps. Moreover, MAEs are controlled below 2 °C for all testing samples, which further verifies the accuracy of the proposed GNN model and temporal prediction method.

4.3. Prediction of thermal stress and displacement

Due to the large span of the bridge, the stress and displacement of some nodes far away from the fire center change little throughout the fire duration. Therefore, according to the position of fire center, a span of 104 m–132 m is submitted to the prediction model. Due to complexity of prediction for mechanical responses, the number of the graph convolution layer is set to 10, and iterations are reduced to 500 or below to avoid overfitting.

Due to the excellent performance in terms of accuracy and efficiency, the embedding method Plan B is employed in this case. The load of the accident vehicle is encoded by $\mathbf{h}_{v_i}^f$. Since the initial node stress and displacement under gravity should be represented as $\mathbf{h}_{v_i}^{init}$, predictions of the stress and deformation are conducted separately. As introduced previously, $\mathbf{h}_{v_i}^{posM}$ contains the distance to the nearest simple supports and distance to the nearest anchorage point considering the constraint effect of the cable. Besides 3 kinds of boundary conditions given in Section 4.2, nodes on simple supports should also be considered and the

dimension of $\mathbf{h}_{v_i}^{bcM}$ is increased to 5. Other input features for thermal prediction are still remained in $\mathbf{h}_{v_i}^M$.

For the stress prediction of the girder, all the 300 testing samples have an accuracy above 90% as shown in Figure 16(a), and the MAPEs of the vast majority of them are lower than 6%. The MSEs of most testing samples are below 5, while only 2 of them have an MSE over 10. In terms of displacement prediction, only 3 testing samples have an MAPE over 10%, accounting for 1% of the testing set. These samples are all generated from two scenarios whose fire areas are located near the simple supports. The percentage error here is mainly contributed by nodes near the simple supports, of which the displacement is close to zero.

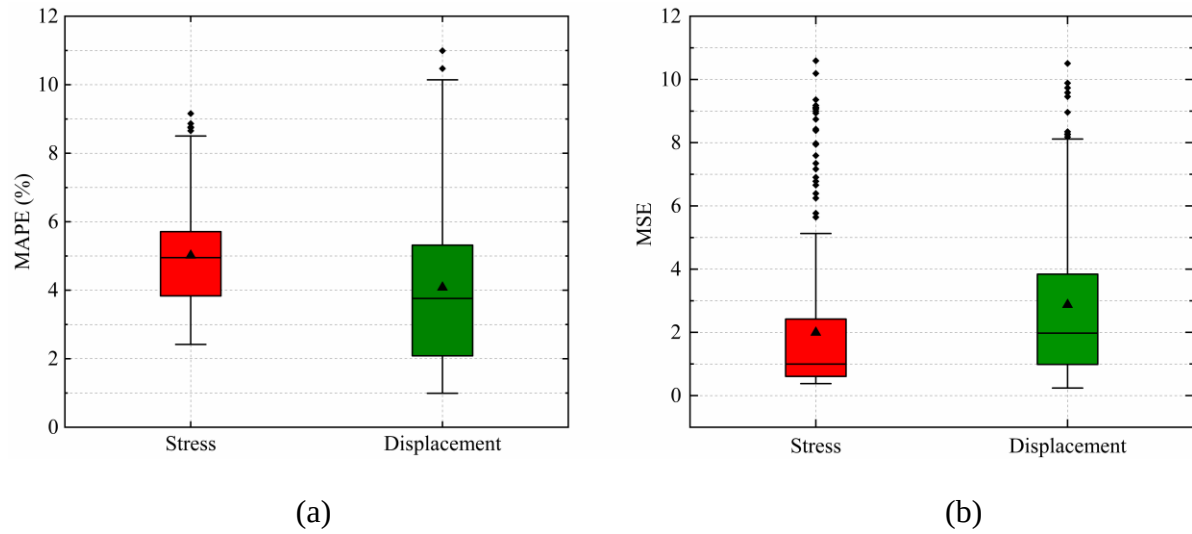


Figure 16. Box plots of (a) MAPEs and (b) MSEs of girder's mechanical response, where the dots indicate the outlier points, the triangles represent the mean errors and black lines in boxes represent the median errors.

In order to verify whether the proposed GNN model can provide correct prediction results at node level, the absolute error distribution of the stress prediction result for a testing sample with a length of 132 m is shown in Figure 17. The GNN model accurately predict the high thermal stress around the fire area of the girder. Since the fire happens on the right side of the bridge, the node stress on right edge of the girder is much larger than that of the other side, and its temporal and spatial distribution is displayed in Figure 18. The largest stress occurs at around 72 m, and the proposed GNN model can accurately predict both the large stress in the middle and lower stress at both ends.

A testing case with a length of 128 m is employed to investigate the performance of the proposed GNN model for displacement prediction at node level. As shown in Figure 19, similar to the slab case, the fire center does not sink but moves upward compared to its original deflection due to the thermal expansion. Instead, the large deflection occurs for nodes around the fire center in the middle of the span because of the strength degradation. Since the deflection at the edge is most noticeable, the true and predicted displacements in the longitudinal direction are compared in Figure 20. It can be observed that the predicted vertical

displacements are in good agreement with the true displacements in both large and small deformation regions.

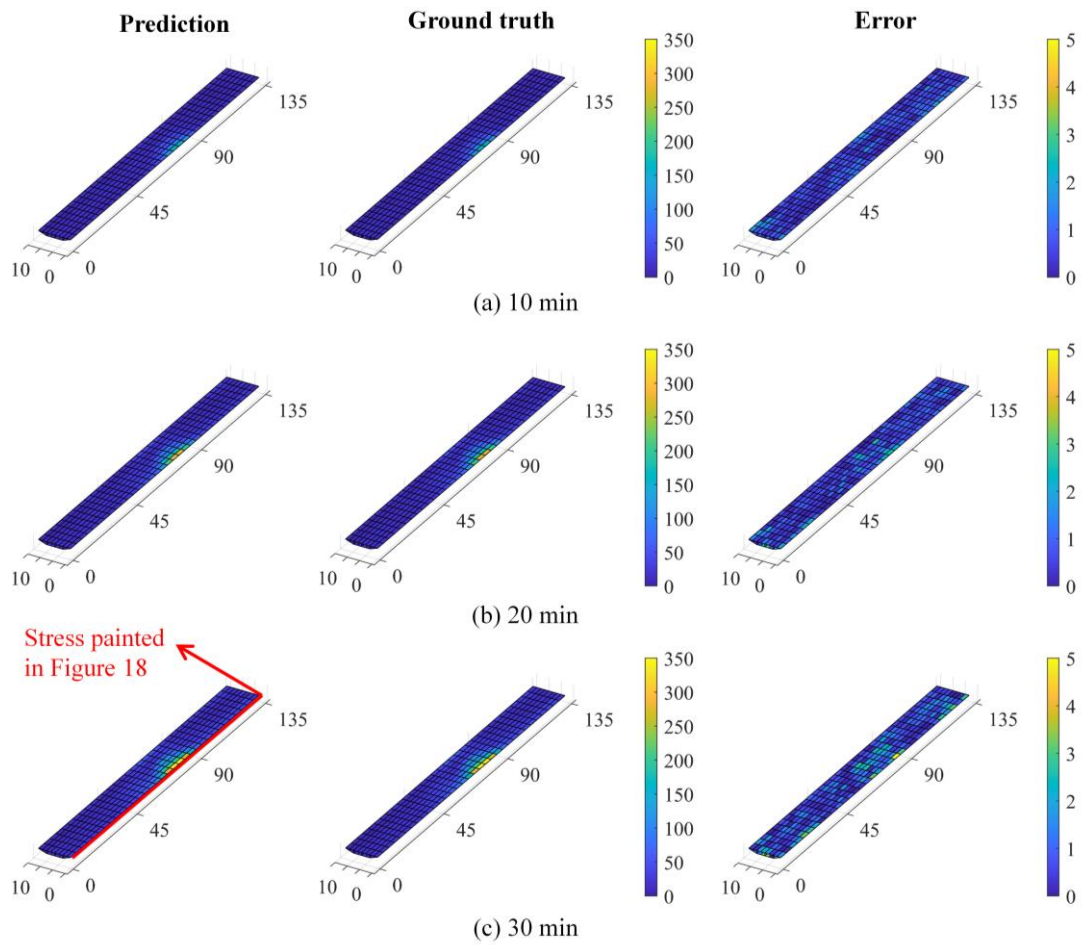


Figure 17. Error distribution in stress prediction at different time steps (length unit: m, stress unit: MPa).

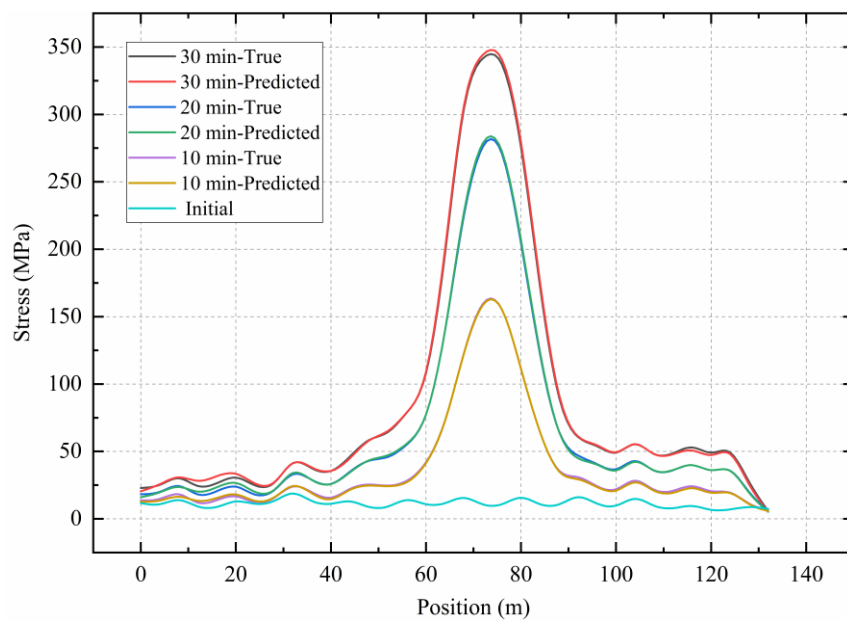


Figure 18. Comparison of predicted and true stresses in longitudinal direction.

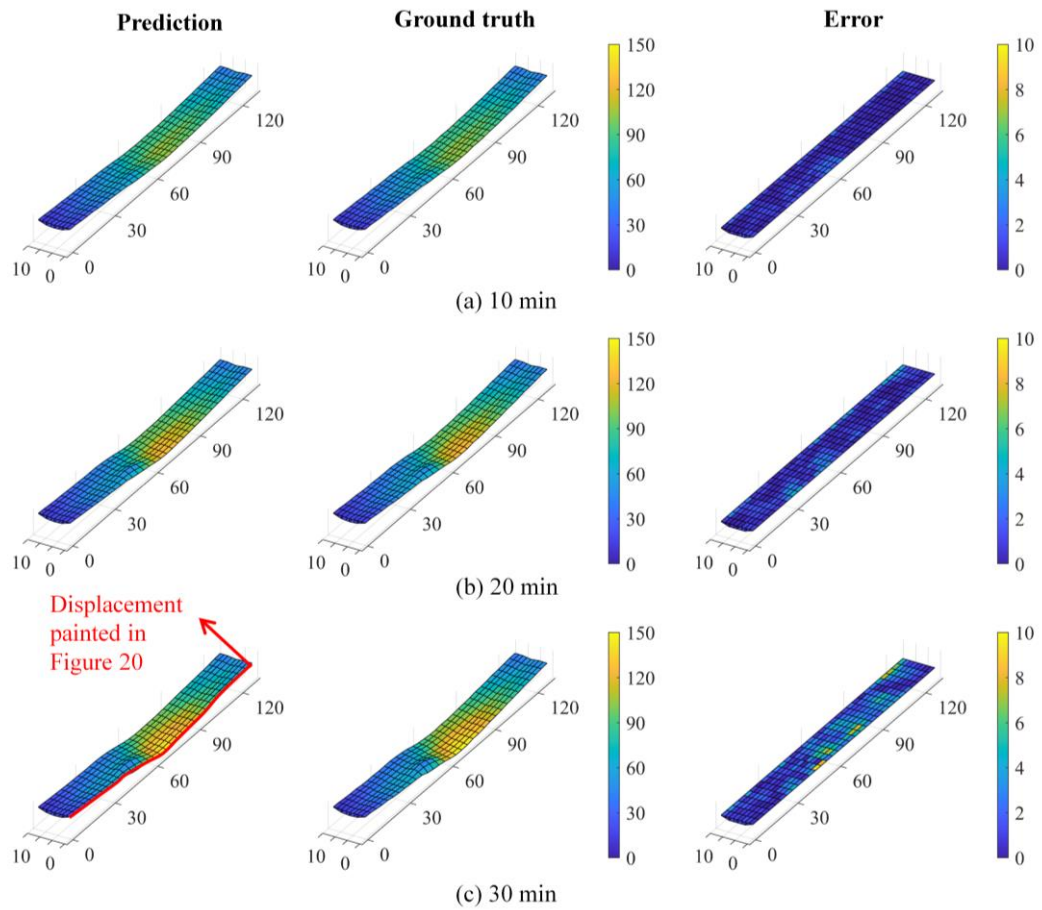


Figure 19. Error distribution in displacement prediction at different time steps, where downward displacement is positive (length unit: m, displacement unit: mm).

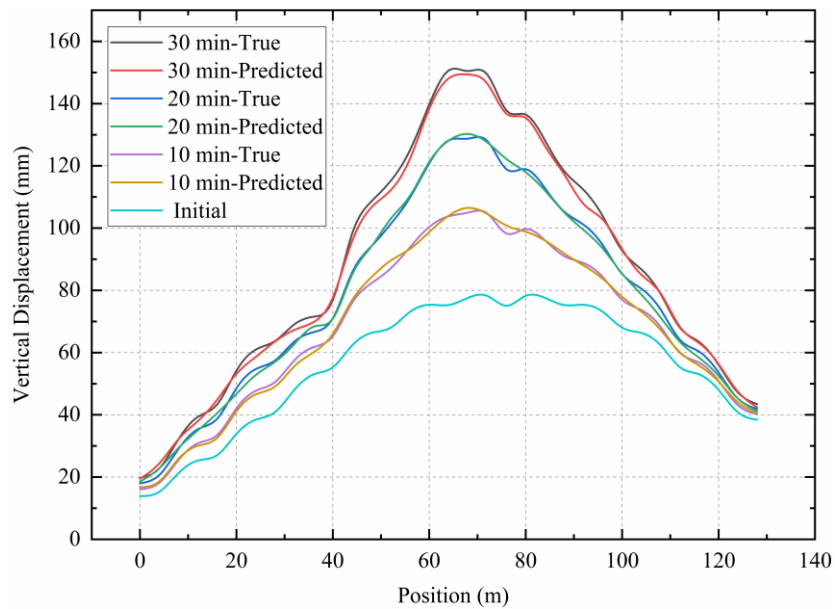


Figure 20. Comparison of predicted and true displacements in longitudinal direction.

4.4. Time efficiency

Although 3 GNNs are used to predict the thermal and mechanical responses for the cable-stayed bridge, the proposed method is much more efficient than the FEM. As shown in Tables 3 and 4, the time consumed by ABAQUS for thermal analysis is 42 times longer than that spent in the proposed GNN model. For the FEM, in order to obtain the stress and displacement at 30 time steps, the temperature field at these steps should be written into different jobs and submitted separately, and thus the total time for the mechanical response prediction is 30 times longer than that for the single-step prediction. GNNs in serial computation mode improve the computational efficiency by over 45 times speedup compared with the FEM for thermo-mechanical prediction. If GNNs operate in parallel, the time required for mechanical prediction and total prediction could be shortened to 24.15 s and 28.81 s, respectively. Consequently, the speedup ratios for the two tasks would increase to 58.47 and 49.01, respectively.

Since the FEM employs a serial computation mode, the computing time of the FEM for mechanical response prediction only is the same as that for prediction of the thermo-mechanical responses. However, the proposed GNN-based method does not require the node temperature as input for mechanical analysis. Therefore, if only the mechanical responses are targeted to be predicted, the advantage of the proposed method in terms of computational efficiency will be more pronounced.

Table 3. Comparison of runtimes in calculating thermal and mechanical response (unit: s).

Method	Temperature	Stress	Deformation	Total
FEM	344.72	$36.58 \times 30 = 1097.4$		1412.12
GNN	8.22	22.33	14.94	45.49

Table 4. Speedup ratio in different tasks.

Task	FEM (s)	GNN (s)	Speedup
Thermal response	344.72	8.22	41.94
Mechanical response	$344.72 + 1097.4 = 1442.12$	$22.33 + 14.94 = 37.27$	38.69
Thermal and mechanical response	1442.12	45.49	31.70

5. Conclusions

A GNN-based framework has been developed in this study for rapid prediction of structural thermo-mechanical responses. A physics-informed aggregate function is designed for the local message passing, enabling the heat conduction to be well captured by the message passing process. For the temperature prediction, two new prediction schemes are proposed to eliminate the effect of error accumulation in the rollout prediction. In terms of the thermal stress and displacement prediction, a new embedding method is introduced, in which the surface heat flux is embedded in the thermal attribute, rather than the predicted node temperature as in conventional methods. Consequently, the proposed GNN model is able to directly predict the stress and displacement, without relying on the previous temperature

prediction results, which further enhances the efficiency and eliminates the error accumulation. If the fire position and heat flux are submitted as input to the proposed GNN model, the node temperature, stress and displacement on time series could be predicted simultaneously.

Two numerical examples are employed to investigate the effectiveness of the proposed prediction model. For the simply supported slab, the proposed two prediction schemes are still able to provide satisfactory results for thermal prediction as the length of the time steps increases, whereas the rollout prediction model cannot. MAPEs of the proposed embedding method are 2.46% and 4.29% for the stress and displacement predictions, which are much lower than those of the conventional method. For the cable-stayed bridge, MAPEs of temperature, stress and displacement predictions are 1.31%, 5.02%, and 4.08%, respectively. Compared with the FEM for thermo-mechanical prediction, the proposed GNN model achieves around 40 and 32 times speedup for the slab and cable-stayed bridge, respectively. Moreover, it is worth mentioning that the numbers of fire scenarios in the training sets are only 122 and 192 for two numerical examples. Through the physics-informed aggregation and innovative embedding, the proposed GNN model is able to provide accurate predictions of thermo-mechanical responses even with a small number of training data, demonstrating its excellent inductive ability.

The results of this study show that the proposed GNN-based framework is able to provide accurate predictions of structural thermo-mechanical responses even for large-scale complex structures, and achieve an order of magnitude speedup compared to the FEM. The proposed method is of high potential for real-time response prediction of large-scale realistic structures during fire emergencies. In future studies, some practical factors, such as the traffic congestion and fluctuation of the heat flux, will be considered to predict thermo-mechanical responses under more realistic and complicated scenarios. Moreover, fire tests are required to further validate correctness of the proposed GNN model.

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Conflicts of interests

The authors declare that they have no known potential conflicts of interest that could have appeared to influence the work reported in this paper.

Authors' contribution

Linghao Kong: Conceptualization, Methodology, Software, Validation, Investigation, Writing – original draft. Rongrong Hou: Conceptualization, Writing – review & editing, Project administration, Funding acquisition. Yuequan Bao: Conceptualization, Writing – review & editing, Supervision, Funding acquisition.

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