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A deep learning-based approach for precision improvement in Monte Carlo neutronics simulation

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ABSTRACT

Neutron flux is a critical parameter in nuclear reactor physics analysis. The Monte Carlo (MC) method is widely used for neutronics simulation due to its high-fidelity modeling capability. However, it suffers from long computation time. Deep learning techniques have demonstrated powerful feature extraction capabilities and high computational efficiency. This study proposes a UNet-based deep learning method with dual-domain data input and hybrid loss function, which uses low-tally MC simulation data as input to reconstruct high-tally results, indirectly enhancing MC neutronics simulation efficiency. The method was validated using 2500 assembly-level total, multi-group neutron flux and pin power distribution dataset generated by OpenMC. Experimental results demonstrated that the model's capability to accurately predict high-fidelity distributions, with prediction residual comparable to or within high-fidelity MC simulation uncertainty and about 167 times acceleration effect. This study highlights the strong potential of deep learning techniques in enabling high efficiency neutronics simulation.

1. Introduction

The neutron flux determines the power distribution within the nuclear reactor core and is an important physical quantity in nuclear reactor design, operation management, and safety analysis. Neutron flux calculation methods are generally classified into deterministic methods and Monte Carlo (MC) stochastic simulation methods. Deterministic methods solve the neutron transport equation numerically by discretization of the spatial, angular, and energy variables. While computationally efficient, the deterministic methods are less adaptable to complex geometries. Moreover, approximation operations such as spatial grid differencing, multi-group cross-section data treatment, and lattice homogenization inevitably introduce calculation errors. In contrast, the MC method, based on stochastic sampling and statistical theory, provides precise modeling of complex geometric structures, physical processes and use continuous energy point-wise cross-section data directly, which can eliminate approximation errors inherent in deterministic methods, and offering greater versatility and flexibility. However, the statistical error in MC simulation is inversely proportional to the square root of the number of particles, requiring a large number of particle transport histories to achieve high precision. This causes high computational costs, slow convergence, and long computation time. Techniques such as variance reduction, scalable parallel computing, and MC-deterministic coupling methods have improved the computational efficiency of the neutronics simulation to some extent (Zhang et al., 2023). Nevertheless, there is still a need for further research into optimization methods to enhance the neutronics simulation performance for high efficiency computing scenario requirements.

Artificial intelligence (AI) technologies, particularly deep learning (DL) (LeCun et al., 2015), have demonstrated remarkable capabilities in extracting abstract features from massive data, facilitating tasks such as detection, recognition, semantic comprehension, and control optimization. DL has achieved significant success in various domains, including computer vision (He et al., 2016), natural language processing (Radford and Narasimhan, 2018), and decision-making systems (Mnih et al., 2015). Its powerful data modeling capabilities and computational efficiency have also revolutionized the scientific computation field. For instance, the DeePMD-kit uses a deep neural network (DNN) to model many-body atomic interactions, successfully simulating quantum molecular dynamics systems with up to 100 million atoms (Wang et al., 2018). The AlphaFold system achieves experimental-level accuracy in predicting protein tertiary structures (Jumper et al., 2021). In the

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nuclear energy field, a wide range of tasks, including reactor core design, fuel management, neutron transport, thermal-hydraulics, radiation shielding, fault detection and diagnosis, entail intensive computation and data analysis. The application of DL methods in these tasks has become an increasingly active and promising area of research nowadays (Huang et al., 2023).

Recent advances have demonstrated the successful application of DL methods for predicting reactor core physical parameters. Zhang et al. developed two convolutional neural network (CNN) surrogate models (VGG-16 and FCN) that use group constant data (in the form of 9 × 9 pixel images) as input to predict the effective multiplication factor k_{eff} (Zhang, 2019), neutron flux and power distributions (Zhang et al., 2021). In another study, Saleem et al. (Abu Saleem et al., 2020) employed a DNN to predict several critical neutronics parameters for large-scale boiling water reactors, including the power peaking factor, control rod bank level, and fuel cycle length. Shriver and Furlong et al. proposed the LatticeNet model that accurately predicts both the normalized pin power distribution and k_{eff} of a fuel assembly using lattice-level physical parameters such as fuel temperature, enrichment, and moderator density as inputs (Furlong et al., 2023; Shriver et al., 2021). Qin et al. (Qin et al., 2020) employed a DNN to generate resonance self-shielded cross-section data. Li et al. (Li et al., 2024) introduced an innovative hybrid architecture combining convolutional and recurrent neural networks, creating a reactor neutron kinetics surrogate model, which can rapidly and accurately predict the reactor core power distribution transients induced by reactivity perturbations.

The aforementioned studies establish DL frameworks to model complex correlations between reactor physics parameters and related data, providing precise predictive capabilities. The two-dimensional neutron flux and pin power distribution can be viewed as a digital image composed of numerous pixels. Given the demonstrated success of DL in image super-resolution (Lim et al., 2017) and de-noising capability (Huo and Yoon, 2021), it holds promise for improving the precision of MC neutronics simulation. Berry and Osborne et al. introduced a CNN-based up-sampling methodology for neutron flux distribution, successfully enhancing the spatial resolution of MC simulation results from 64 × 64 pixels to 128 × 128 pixels while simultaneously increasing the number of energy groups from 8 to 16. This method exhibits robust applicability across diverse reactor configurations, encompassing variations in fuel pin quantities, enrichment levels, and burnup conditions (Berry et al., 2024a, 2024b; Osborne et al., 2023). Yuan et al. (Yuan et al., 2023) proposed a hybrid CNN-Transformer architecture for low-dose Computed Tomography (CT) image denoising that can effectively preserve image details while suppressing noise artifacts. Ardakani et al. (Raayai Ardakani et al., 2022) developed a cascade CNN model that can improve the quality of MC simulation results for near-infrared photon imaging, reduce the simulation time, and their study also validates that DL denoising methods outperform traditional model-based denoising methods. Liu et al. (Liu et al., 2025) proposed a CNN and parallel Transformer hybrid network model that can reduce the blur problem in neutron imaging and enhance the performance of neutron cameras.

The previous studies aiming to improve the precision of neutron flux distribution or image data based on DL methods (by up-sampling and denoising) only used spatial domain data as input, ignoring the frequency spectrum features. The frequency spectrum provides a mathematical representation of spatial data in the frequency domain, providing critical information about the periodicity, texture, and edge features, which is valuable for data compression, denoising, and detail recovery application (Sundararajan, 2017). To leverage the spectral features of neutron flux or pin power distribution and fill the research gap, this study proposes a novel dual-domain UNet framework for improving the precision of MC neutronics simulation at fuel assembly level. The UNet architecture is selected, which is originally developed for biomedical image segmentation (Ronneberger et al., 2015), has down-sampling (encoder) and up-sampling (decoder) modules, with a structure resembling the letter "U". It has skip connections, which enables effective processing of hierarchical feature information, enhance the feature extraction and reconstruction capability. Dual-domain data refers to the low-precision neutron flux or pin power distribution data in both the spatial domain and its frequency spectrum. In addition, a hybrid loss function of mean squared error (MSE) and structural similarity index measure (SSIM) is used to guide the optimization of model parameters (weights and biases in the network layers). The MSE component considers the prediction error of all pixel points, while the SSIM evaluates global structural similarity between predicted and target distributions (the ground truth). The integration of both metrics is expected to improve the model's learning efficiency and predictive performance.

This study presents a new idea for high-efficient calculation of neutron flux and pin power distribution based on the integration of MC simulation with DL methods. The main contribution of this work is summarized as follows: 1) introduction of dual-domain data input for UNet model to capture both spatial and spectral characteristics; 2) design of a hybrid loss function for balancing local and global accuracy metrics; 3) develop an effective DL model for MC neutronics simulation precision improvement. The remainder of this paper is organized as follows: Section 2 introduces the research dataset, proposed new method, model training process and evaluation metrics. Section 3 analyzes the model training convergence, prediction results and errors vs. high-precision MC simulation in various scenarios, and the influence of different model input, loss functions, and training sample scales on model performance. Section 4 summarizes the research results and discusses potential directions for future study.

2. Materials and methods

2.1. Research dataset

The OpenMC (v0.15.0) (Romano et al., 2015), an open-source MC particle transport simulation code developed by Massachusetts Institute of Technology and the scientific community, is selected as the computational tool for neutron flux and pin power calculation in this study. First of all, the fuel assembly model is constructed. The fuel assembly has a square shape with a side length of 21.42 cm, containing 289 (17 × 17) cells. The pitch of two adjacent cells is 1.26 cm. Then ten cells are randomly selected to place the control rods (the material is Ag-In-Cd alloy), while the rest cells are filled with UO_2 fuel rods (encased in zirconium alloy cladding), having varying enrichment of ^{235}U with 1.8 %, 2.4 %, 3.1 %, 4.0 % and 4.8 %. The rest space of the assembly model is filled with water as the neutron moderator material.

2500 assembly cases were randomly generated and each enrichment contains 500 cases. Depletion simulation was performed to obtain neutron flux and pin power data for fresh and depleted fuel assembly. The "chain_simple.xml" file provided by the official OpenMC GitHub repository was used to determine the paths by which nuclides transmute over the depletion simulation. Referring to the related study and official code example (OpenMC, n.d.), the fuel line power density was set to 174 W/m (Berry et al., 2024a), and the first-order predictor algorithm is selected as time-integration algorithm for depletion calculation with a time step of 10 days. The simulations reached a maximum burnup of approximately 1.496 MWd/kgIHM. The ENDF/B-VII.1 library was used as the nuclear cross-section database. The geometry tally mesh was set to 128 × 128. For multi-group neutron flux calculation, the energy filter was set up with energy bins of 0, 0.001 eV, 0.1 eV, 0.625 eV, 1 eV, 6.25 keV, 100 keV, 5.5 MeV, 20 MeV to get eight-group neutron flux tallies.

Each simulation used 20 inactive cycles followed by 80 active cycles, with 10^3 and 10^6 particles per cycle to obtain total neutron flux, multi-group neutron flux, and pin power distribution data at the initial and four subsequent depletion steps, respectively. The standard deviations of these tallies were also recorded to reflect the statistical uncertainty of the MC simulation. Simulation results with 10^3 particles per cycle are considered as low-precision data, which will be used as model input.

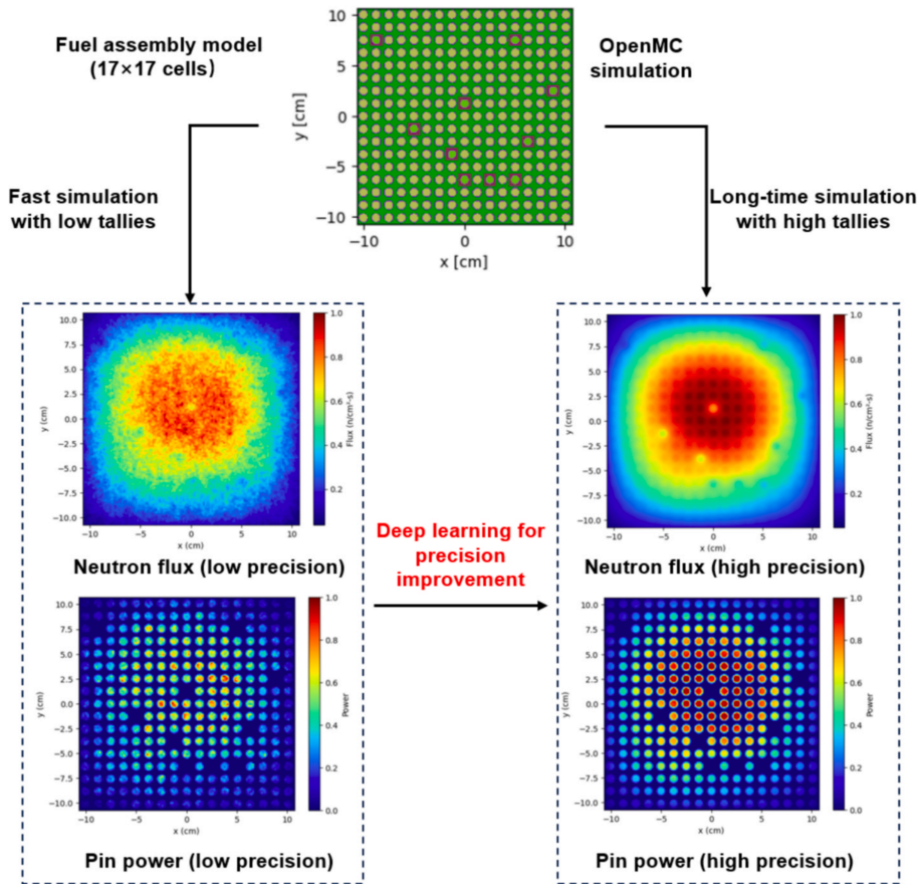

Fig. 1. A fuel assembly modeled using OpenMC and its simulation results of neutron flux and pin power distribution with different precision levels.

Simulation results with 10^6 particles per cycle are considered as high-precision reference data, serving as training label (i.e., the ground truth). The fuel assembly model constructed in OpenMC, along with the simulation results of neutron flux and pin power distributions with low and high precision are shown in Fig. 1. The neutron flux and pin power distribution results are pre-processed by 0–1 normalization for model training and testing.

In this study, the Fast Fourier Transform (FFT) (Buijs et al., 1974) is used to convert the neutron flux or pin power distribution from the spatial domain to the frequency domain using the following equation:

$$F(u,v) = \sum_{x=0}^{M-1} \sum_{y=0}^{N-1} f(x,y) e^{-j2\pi(ux/M+vy/N)} \tag{1}$$

where F is the frequency spectrum. f is the spatial distribution data. u and v are the frequency variables. x and y are spatial coordinates. M and N denote the width and height of the distribution data matrix, respectively. j is the imaginary unit. The frequency spectrum captures essential features of distribution data. Generally, the low-frequency components correspond to the slowly varying regions, such as flat areas, while the

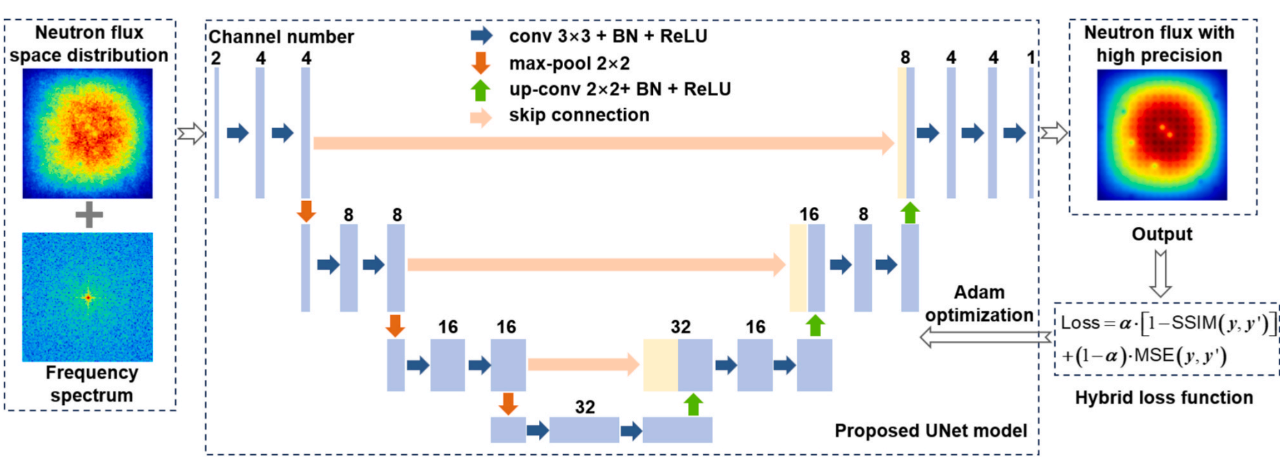

Fig. 2. The proposed dual-domain UNet model with hybrid loss function. Here, total neutron flux prediction model is shown as example. For pin power prediction model, the input and output label are substituted as pin power data while the model architecture keeps the same. The numbers above the network layer refer to the channel number.

Table 1
Key information of the proposed UNet model.

Module	Hyperparameter	Value
Input layer	Input data shape	[n, c_1, 128, 128]
Encoder	Conv block #1 and #2	Conv: 4@3 × 3, padding = 1 Batch normalization layer ReLU activation
	Pooling layer #1	Max pool: 2 × 2 stride: 2 × 2
	Conv block #3 and #4	Conv: 8@3 × 3, padding = 1 Batch normalization layer ReLU activation
	Pooling layer #2	Max pool: 2 × 2 stride: 2 × 2
	Conv block #5 and #6	Conv: 16@3 × 3, padding = 1 Batch normalization layer ReLU activation
	Pooling layer #3	Max pool: 2 × 2 stride: 2 × 2
	Conv block #7 and #8	Conv: 32@3 × 3, padding = 1 Batch normalization layer ReLU activation
Decoder	TransConv block #1	TransConv: 16@2 × 2, stride = 2 × 2 Batch normalization layer ReLU activation
	Conv block #9 and #10	Skip connection from conv-block #6 Conv: 16@3 × 3, padding = 1 Batch normalization layer ReLU activation
	TransConv block #2	TransConv: 8@2 × 2, stride = 2 × 2 Batch normalization layer ReLU activation
	Conv block #11 and #12	Skip connection from conv-block #4 Conv: 8@3 × 3, padding = 1 Batch normalization layer ReLU activation
	TransConv block #3	TransConv: 4@2 × 2, stride = 2 × 2 Batch normalization layer ReLU activation
	Conv block #13 and #14	Skip connection from conv-block #2 Conv: 4@3 × 3, padding = 1 Batch normalization layer ReLU activation
	Conv block #15	Conv: 1@3 × 3, padding = 1 Batch normalization layer ReLU activation
Output layer	Output data shape	[n, c_2, 128, 128]
Model training	Optimizer	Adam
	Loss function	Proposed mixed loss function of SSIM and MSE with $\alpha = 0.2$, shown in Eq.(2)
	Learning rate	0.001
	Batch size	32
	# of epoch	50

Note: [n, c, 128, 128], n indicate number of samples. c refers to the input or output channel. $c_1 = 2$, $c_2 = 1$ for neutron flux and pin power prediction model. $c_1 = 16$, $c_2 = 8$ for multi-group neutron flux prediction model. [128, 128] refers to the input data matrix height and width. Conv refers to the convolution operation. TransConv refers to the transposed convolution operation, which can up-sample the resolution of input feature maps.

high-frequency components represent rapid changes and fine details, such as edges and discontinuities. In this study, the frequency spectrum is incorporated as additional input to the DL model to provide rich frequency features of the neutron flux and pin power distribution. This dual-domain representation is expected to improve the model's ability to learn and generalize complex patterns in neutron flux and pin power distributions.

2.2. Proposed dual-domain UNet model

In this study, a dual-domain input UNet model is proposed for precision improvement of MC neutronics transport simulation, as illustrated in Fig. 2. The model establishes an end-to-end mapping between the low-precision neutron flux and pin power distribution data (generated from low-tally MC simulation) and their high-precision counterparts (generated from high-tally MC simulation) by leveraging joint feature learning and reconstruction in both the spatial and frequency domains.

The backbone of the proposed model is a UNet architecture, comprising an encoder module and a decoder module. The encoder module progressively reduces the spatial resolution of the input data, while increasing the number of feature channels, enabling hierarchical feature extraction through a sequence of 3 × 3 convolution, batch normalization (BN), rectified linear unit (ReLU) nonlinear activation, and 2 × 2 max-pooling operations. The decoder module achieves up-sampling through transposed convolution operations to restore the spatial resolution of the feature maps, while reducing the channel capacity. The feature maps have skip connections between the encoder module and the corresponding levels of the decoder module to retain contextual information for enhancing the detailed features restoration and reconstruction capability. The dual-domain data provides both spatial distribution and spectral information, which enriches the model learnable information to establish more comprehensive and deeper mapping relationships, ultimately improving predictive performance. Detailed computational operations in different kind of network layers could be found in many DL tutorials or research papers, so they are not described here for brevity.

The hybrid MSE and SSIM loss function are set as follows:

$$\text{Loss} = \alpha \cdot [1 - \text{SSIM}(y, y')] + (1 - \alpha) \cdot \text{MSE}(y, y') \tag{2}$$

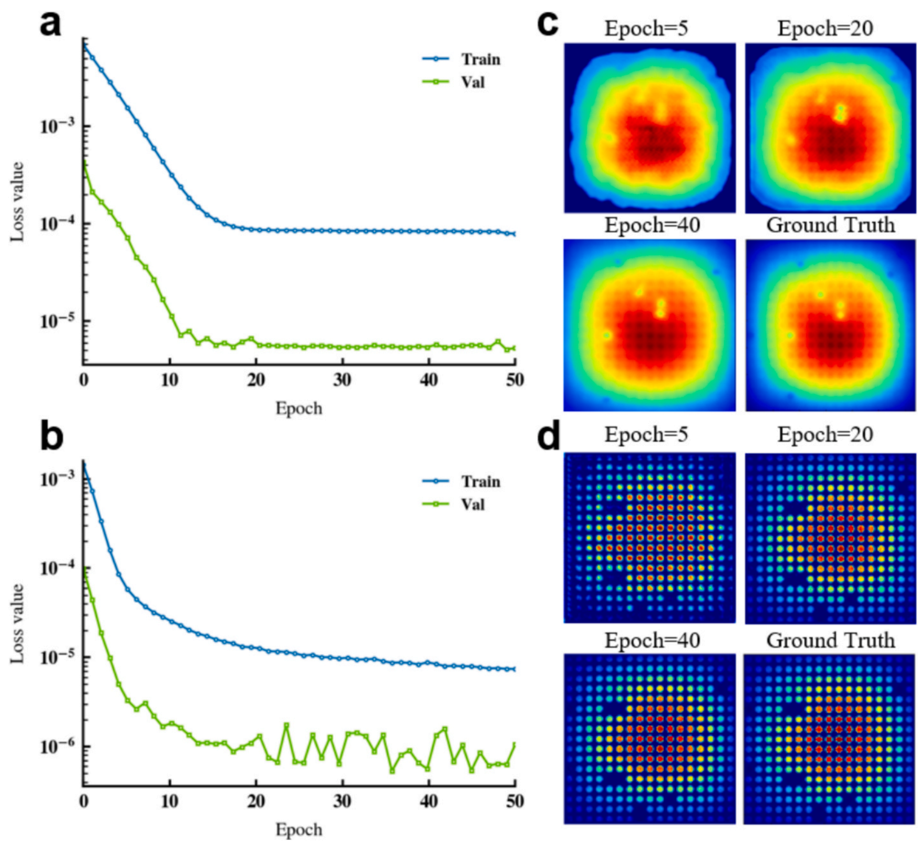

Fig. 3. Analysis of the proposed model training process: loss curves of (a) neutron flux and (b) pin power prediction; the predicted outputs at different training stages of (c) neutron flux and (d) pin power prediction. For loss value curve, the y-axis is presented on a logarithmic scale.

where y denotes the labeled data and y' denotes the model prediction. α is the weight coefficient, which controls the relative contribution of different loss components. The SSIM evaluates the similarity between two distribution data in three aspects, i.e., brightness, contrast and structure, which aligns well with human visual perception, and is commonly used to evaluate the quality of image compression, enhancement and denoising (Wang et al., 2004). The SSIM is calculated as follows:

$$\mathrm{SSIM}(x,y)=\frac{(2\mu_x\mu_y+C_1)(2\sigma_{xy}+C_2)}{(\mu_x^2+\mu_y^2+C_1)(\sigma_x^2+\sigma_y^2+C_2)} \tag{3}$$

where μ denotes the mean value, reflecting the average intensity of an assembly flux or pin power distribution. σ^2 denotes the variance of the flux or pin power tally values, reflecting the contrast. σ_{xy} denotes the covariance of flux or pin power tally matrix x and y, reflecting the structural similarity. C_1 and C_2 are constants to prevent division by 0 in the denominator. A SSIM value closer to 1 signifies a higher similarity between the two flux or pin power distribution, while a value closer to 0 indicates a lower similarity between them.

The MSE is shown as follows:

$$\mathrm{MSE}(x,y)=\frac{1}{MN}\sum_{i=0}^{M-1}\sum_{j=0}^{N-1}[x(i,j)-y(i,j)]^2 \tag{4}$$

where M and N denote the width and height of the data matrix, respectively. $x(i,j)$ denotes the pixel values in data x (neutron flux or pin power distribution) with coordinates of i and j. The hybrid loss function integrates the prediction error of pixel-wise data and the overall structural similarity of the distribution data to guide the model parameter update and feature extraction more efficiently.

2.3. Model training and evaluation

In this study, 2500 assembly cases were simulated by the OpenMC code (v0.15.0), which are then randomly divided into three parts in the ratio of 50 %:20 %:30 %, constituting the training set, validation set and test set, respectively. The data (neutron flux and pin power distribution) of fresh, depleted assemblies account for 20 %, 80 % (including 4 burnup steps) within each sub-dataset (i.e., training set, validation set and test set), respectively. The training set is used for model fitting. The validation set monitors loss value convergence during training. The test set is not involved in model training and optimization, which is only used for evaluating model performance. To mitigate the influence of sample division randomness, the model's average performance across 20 independent random test splits is reported as the final evaluation result.

The proposed model was developed using the popular DL development framework PyTorch (v2.0.1) (Paszke et al., 2019). The total, multigroup neutron flux and pin power prediction model were built separately, with same network architecture but different input/output data types. Model hyperparameters were set by developing experience and trial. The input of the model is 128×128 normalized neutron flux or pin power distribution data and its frequency spectrum. The number of feature channels in the internal hidden layers is shown above each network layer in Fig. 2 and summarized in Table 1. The Adam optimizer (Kingma and Ba, 2015) is used for model training and parameter updating, with an initial learning rate of 0.001. The hybrid loss function parameter α is set as 0.2 according to the performance test. In every training epoch, 32 samples are used as a mini-batch for stochastic gradient descent optimization. The key information of the proposed UNet model and its training strategy are summarized in Table 1. The unmentioned model parameters (such as the initial parameter setting of network layers and the Adam optimizer) were used with the default settings in the PyTorch developing framework. For engineering

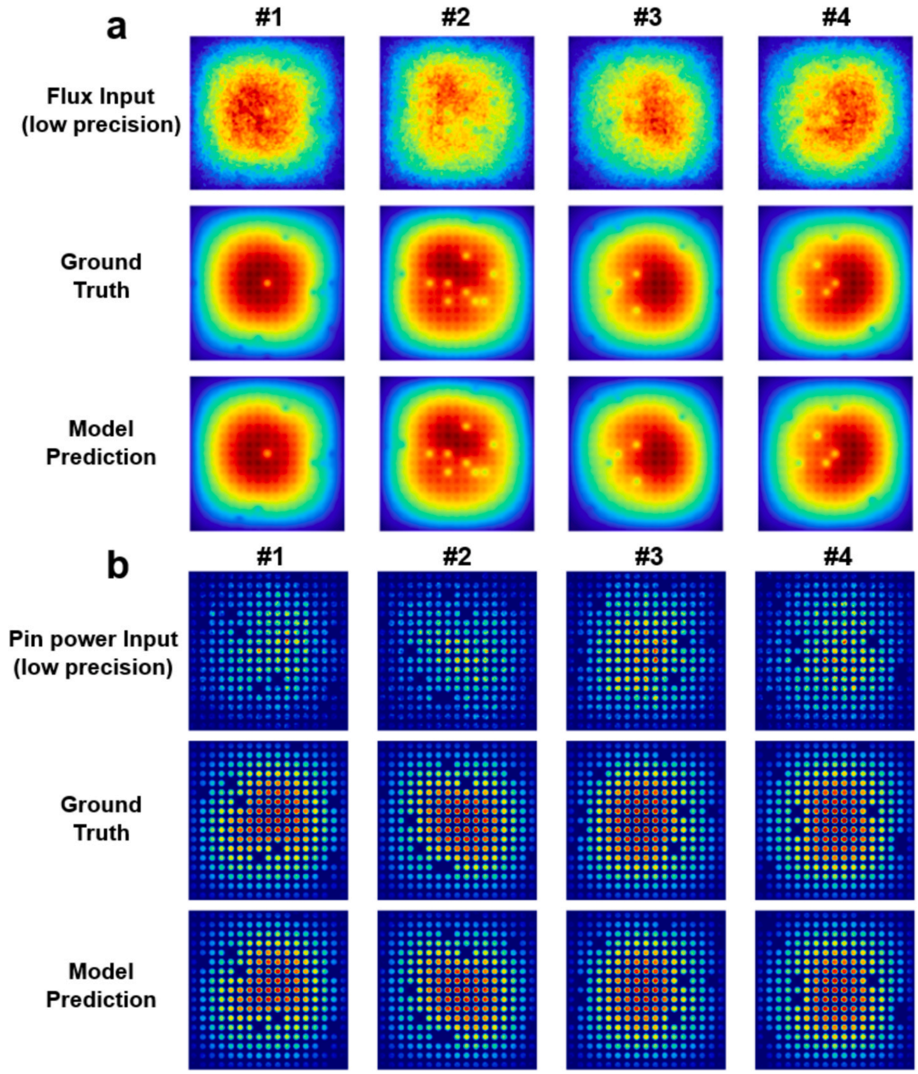

Fig. 4. Prediction results of the proposed UNet model on four randomly selected cases from (a) total neutron flux test data and (b) pin power test data.

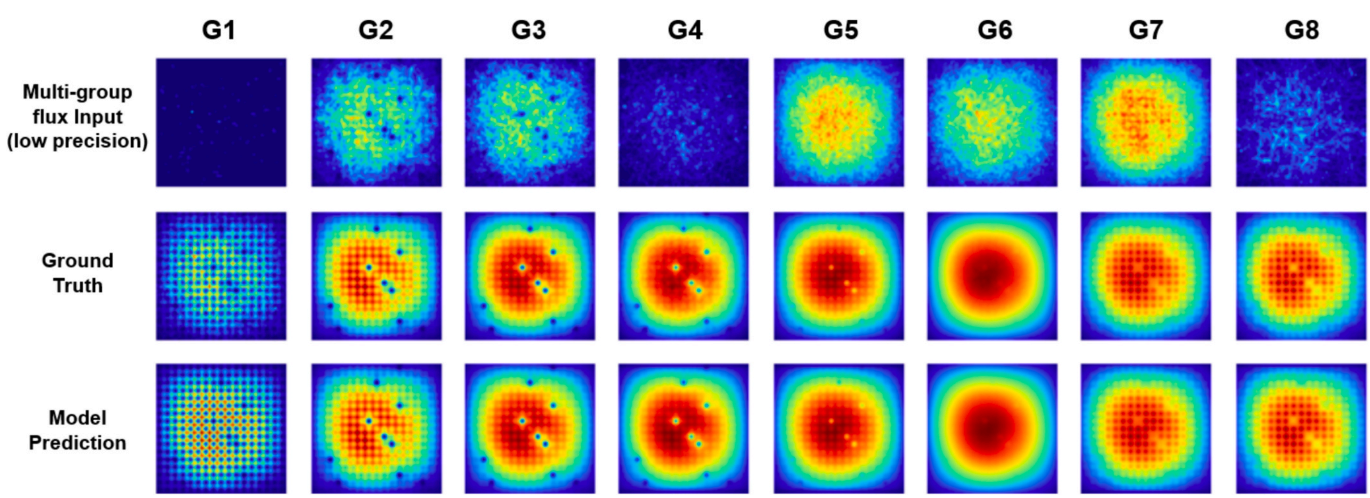

Fig. 5. Prediction results of the proposed UNet model on one case from the multi-group neutron flux test data. G1 ~ G8 denote the different energy groups.

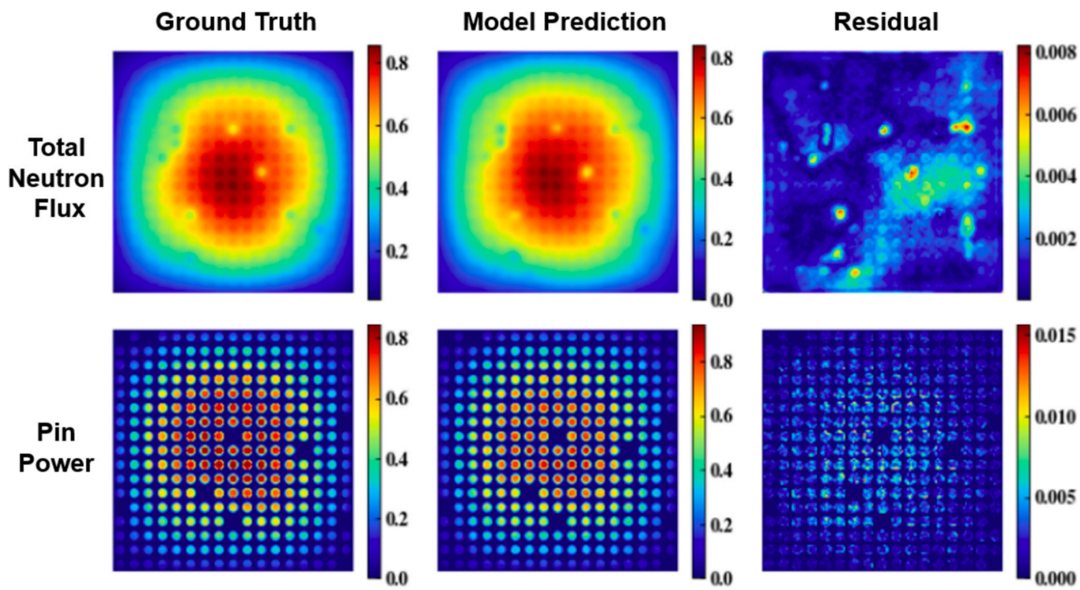

Fig. 6. Residual distributions between model predictions and high-precision MC simulation. Notably, flux prediction errors are more significant near control rod positions.

Table 2
The prediction errors of the proposed UNet model against Monte Carlo uncertainty.

Data		MAE of the model predictions vs. high-precision MC simulation results	Standard deviation (uncertainty) of high-precision MC simulation results
Pin power		0.00112	0.00108
Total neutron flux		0.00133	0.00129
Multi-group	G1	0.00439	0.00432
neutron	G2	0.00233	0.00347
flux	G3	0.00324	0.00462
	G4	0.01256	0.01005
	G5	0.00275	0.00238
	G6	0.00269	0.00338
	G7	0.00151	0.00154
	G8	0.00812	0.00903

Note: MAE = mean absolute error. MC = Monte Carlo. G1 ∼ G8 denote the different energy groups.

application, model structure parameters and training strategy can be further optimized to improve its performance. This study aims to provide a preliminary exploration of the feasibility and computational performance of the proposed method. On the other hand, DL model optimization is an open issue and under ongoing research. Therefore, the model hyperparameter optimization is not discussed in this work.

The SSIM and mean absolute error (MAE) are used as model performance evaluation metrics. The definition of SSIM is given in the previous section and defined in Eq (3). The MAE is calculated as follows:

$$\mathrm{MAE}(x,y)=\frac{1}{MN}\sum_{i=0}^{M-1}\sum_{j=0}^{N-1}|x(i,j)-y(i,j)| \tag{5}$$

where M and N denote the width and height of the data matrix, respectively. $x(i,j)$ denotes the values in data x (neutron flux or pin power distribution) with coordinates of i and j. A lower MAE indicates higher prediction accuracy.

3. Results and discussion

3.1. Analysis of the model training process

Fig. 3(a) and (b) show the model loss value curve in the training set (i.e., training loss) and validation set (i.e., validation loss) during the iterative training process for neutron flux and pin power prediction, respectively. Both loss curves exhibit a clear downward trend followed by convergence indicating effective training. After each training epoch, model performance is evaluated in the validation dataset. Since the training process improves the model's prediction capability and the validation set has similar features with the training dataset, the validation loss at the end of each epoch is less than the training loss. When the epoch reaches 20, both the training loss and validation loss values tend to stabilize and converge. At the end of model training, the training loss reaches the order of 10^{-4} and the validation loss reaches the order of 10^{-5} in neutron flux prediction scenario; the training loss reaches order of 10^{-5} and the validation loss reaches the order of 10^{-6} in pin power prediction scenario. Fig. 3(c) and (d) show the prediction results for the same sample at different training stages. The prediction results gradually approach the ground truth as the training proceeds, which also indicate that the proposed model converges well in neutron flux and pin power dataset after training given by the hyperparameter setting in this work.

3.2. Prediction results and error analysis

Fig. 4 shows the prediction results of the proposed method on four randomly selected samples in the neutron flux and pin power test dataset, respectively. Fig. 5 shows the prediction results of the proposed method on one randomly selected case from multi-group neutron flux test dataset. These predictions are very close to the high-precision MC

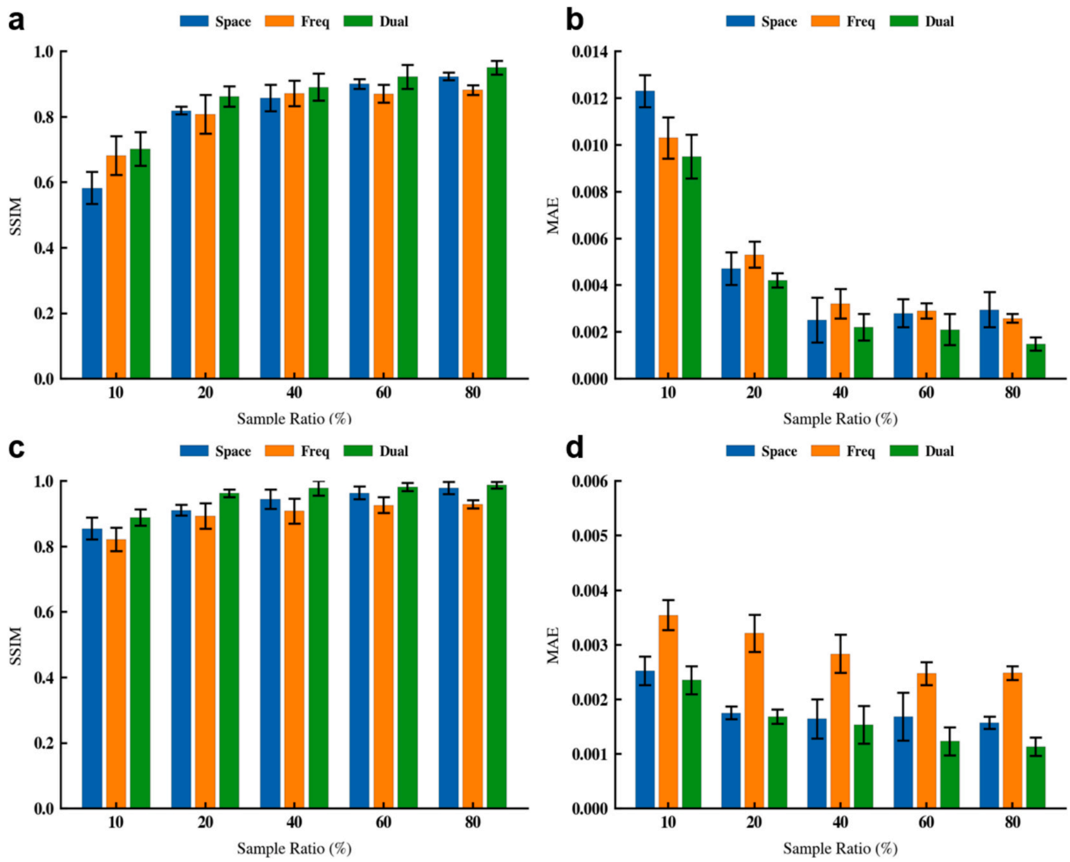

Fig. 7. Model prediction performance under different inputs and training sample scales. (a)(b) for neutron flux prediction; (c)(d) for pin power prediction. SSIM = structural similarity index measure), MAE = mean absolute error. “Space” denotes the spatial distribution of neutron flux or pin power data as model input; “Freq” denotes the frequency spectrum; “Dual” means both the spatial and spectrum data are used as model input (two input channels).

simulation results, indicating that the model can be well trained and converged under the given dataset, model parameters and training strategy. The proposed method is expected to achieve the precision improvement of the low-tally MC simulation results and has potential to significantly reduce the high-fidelity MC neutronics simulation time.

The high-precision neutron flux and pin power distribution data obtained from high-tally MC simulations are used as the ground truth to calculate the deviations (or called residual) of the model predictions. Fig. 6 shows the model prediction results, high-precision MC simulation results and their absolute residual distribution. For the neutron flux prediction task, larger residuals are observed near the control rod positions. The possible reason is that the control rod is a strong absorber of neutron, which introduces sharp spatial gradients in flux near the interface, making the model prediction accuracy deteriorates. The rest of the neutron flux distribution is more uniform, and the model prediction accuracy is good. The pin power prediction errors are mainly distributed at the fuel rod location, especially at the assembly center with higher power.

Table 2 summarizes the model prediction MAE versus the high precision MC simulation results, and the tally standard deviation (uncertainty) of the high precision MC simulation for various scenarios of pin power, total neutron flux, and multi-group neutron flux data. In all experiment cases, the model predictions are close to or less than the statistical standard deviation (uncertainty) of the MC simulation, indicating that the proposed UNet model reaches or approaches the level of high-precision MC simulations, and has the potential to combine the low-precision MC simulation results to reconstruct the high-fidelity results, significantly improving neutronics simulation efficiency.

The pin power, neutron flux data are normalized to the range of $0 \sim 1$ in this study.

Next, we compare the predictive capability of the well-trained UNet model when making predictions using fresh and depleted fuel assemblies. The fresh and depleted fuel data in the test dataset are separated and the model prediction results are also counted separately. The flux prediction MAE in the fuel and depleted assemblies are 0.00132 and 0.00133, respectively. The pin power prediction MAE in the fuel and depleted assemblies are both 0.00112. Results show that the proposed model can make good predictions under fresh and depleted fuel assembly data. The possible reasons for this phenomenon are: 1) the proposed model is trained in a mixture of fresh and depleted assembly data, which allows it to learn and capture data features and patterns of fresh and depleted assemblies; 2) The burnup level used in this study is relatively small ($0 \sim 1.496$ MWd/kgIHM), and the similarity between the train and test data in different burnup steps is high, which reduces the challenge of the model predictions. In the neutron flux prediction scenario, the model predictive capability is relatively a little poor, which indicates that burnup makes the data features a little more complicated.

3.3. *Influence of model input and loss function*

In this study, dual-domain (spatial and frequency spectrum) data inputs and hybrid loss function (MSE + SSIM) are presented. This section discusses the influence of different model inputs and hybrid loss function weight parameter on model performance. Three types of input data and five different training sample scales are considered in this experiment. The low-precision total neutron flux and pin power spatial distribution data, frequency spectrum, and dual-domain (both the spatial and frequency spectrum, as two input channels) data are used as model inputs, respectively. Fig. 7 shows the histogram of the model prediction performance metrics SSIM and MAE. As the training set size

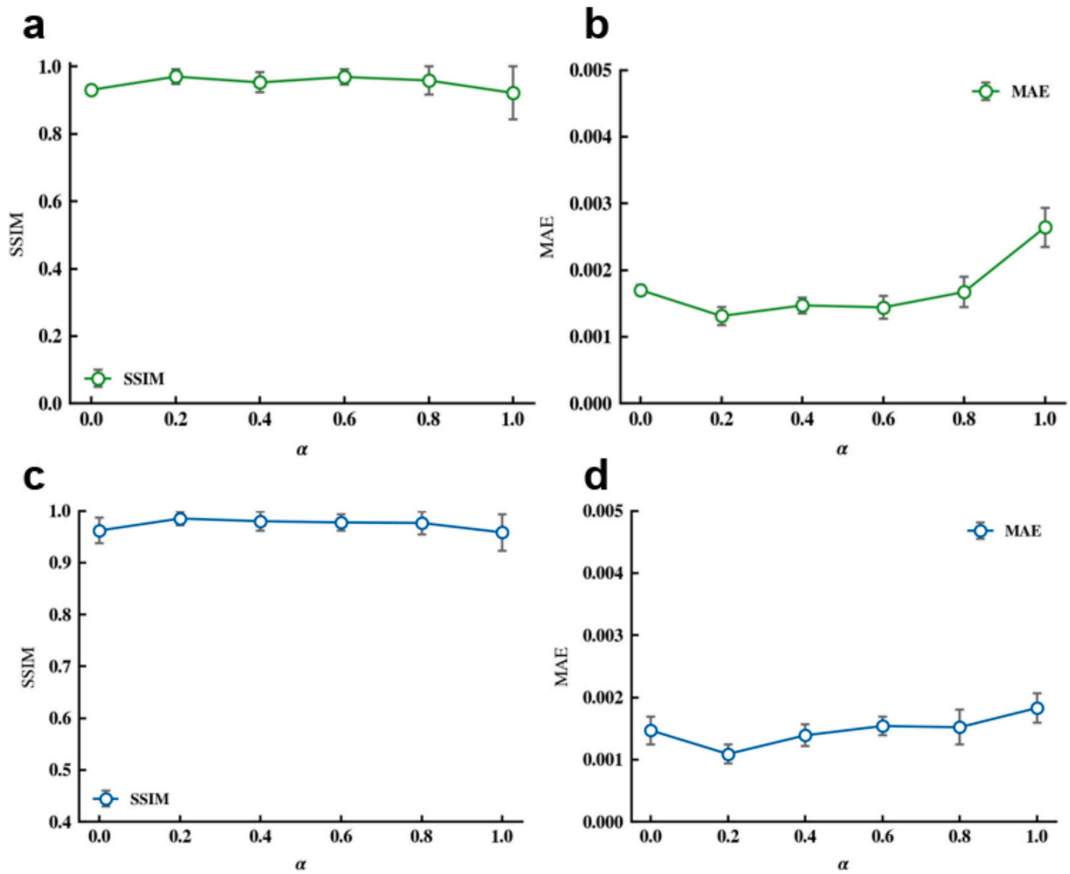

Fig. 8. Influence of weight coefficient in the hybrid loss function on model performance. (a) (b) for neutron flux prediction; (c)(d) for pin power prediction. SSIM = structural similarity index measure, MAE = mean absolute error.

increases from 10 % to 80 % of the original size, both the predictive performance metrics show an improving trend. This improvement can be attributed to the model's enhanced capacity to capture feature representations through progressively enriched training samples, consequently yielding superior generalization performance on the test data sets. This phenomenon aligns with fundamental deep learning principles regarding data-driven model optimization.

Across all experimental configurations, the model with dual-domain data input consistently demonstrated superior performance compared to the models utilizing single-domain data as input. The observed performance advantages may stem from the complementary feature representation enabled by dual-domain feature learning, which effectively combines spatial and frequency patterns. This synery of heterogeneous data domains provides richer features, which are particularly beneficial for improving reconstruction fidelity. For the pin power prediction scenario, the SSIM metric are better than the neutron flux prediction experiments. This may be attributed to the more regular and structured nature of pin power distributions, with large power at the fuel rod cell elements and near-zero values at other locations. Therefore, the pin power distribution patterns can be more easily learned and predicted by the UNet model.

The DL model training process aims to minimize the training loss function by employing the stochastic gradient descent method to iteratively optimize the weight and bias parameters. The loss function design has influence on the model optimization direction and final performance. While the MSE loss function captures the prediction error of all pixel values, it is insensitive to structural similarity in the overall spatial distribution. To address this limitation, this study introduces a mixed MSE and SSIM loss function, as shown in Eq. (2), to enhance the model's capability for global and local error optimization. Here, different α values are set to analyze its impact on the model performance. Fig. 8

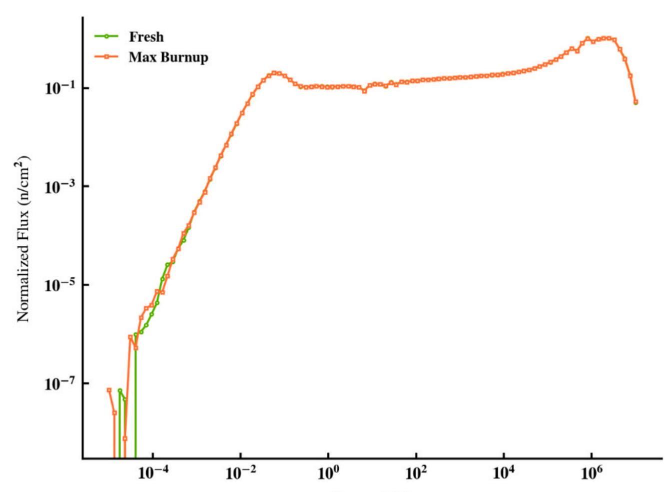

Fig. 9. The neutron flux spectrum between fresh and depleted assembly with maximum burnup level in this study. Logarithmic coordinates are used for both the x- and y-axes.

shows the SSIM and MAE of the model predictions for different cases. When α is 0 or 1, the hybrid loss function degenerates to a single loss function (i.e., MSE or SSIM). The results show that he hybrid loss function makes model perform a little better. In this study, when α is 0.2, the model has best performance with SSIM reaching 0.9703 (in total neutron flux prediction experiment) and 0.9851 (in pin power prediction experiment), MAE reaching 0.0013 (in total neutron flux prediction experiment) and 0.0011 (in pin power prediction experiment). Therefore, $\alpha = 0.2$ is selected for the model setting.

3.4. Related discussion

Based on the principle of DL data noise reduction, this study proposes a dual-domain input UNet model with hybrid loss function to realize the precision improvement of neutron flux and pin power calculation at fuel assembly level. The proposed method leverages low-tally MC simulation results as inputs to predict high-tally simulation results, significantly reducing the computational cost while maintaining high accuracy. The experiment results in Section 3.2 verify that the method's predicted errors are close to or within the computational uncertainties of high-fidelity MC simulation, validating the effectiveness of the proposed method.

Now, we analysis the computation time of different methods. One of the computing servers in our laboratory is used as an example, which has an Intel(R) Xeon(R) CPU E5-2630 with 20 cores and a GPU card (NVIDIA GeForce GTX 1080 Ti). The code running tests show that a low-precision MC simulation takes about 4.39 s, and a high-fidelity MC simulation takes about 731.20 s. Training the proposed UNet model takes about 56.7 s. Generally, when the model training is completed, it can be saved permanently as a file and used for similar tasks directly without retraining. In the application stage, only the model prediction time is considered. The model prediction time takes about 0.0002 s for one case, which is very fast and negligible compared to the low-precision MC simulation time. So, the proposed method can obtain accurate high-precision simulation results with just the time spent on the low-precision MC simulation results, which achieves a computational acceleration effect of about 167 times. The DL has a strong potential for application in high efficiency reactor neutronics computation.

The k_{eff} is also a very crucial system-level physical quantity in reactor neutronics analysis, which reflects the neutron multiplication properties of the fuel system. We tried $\mathrm{k_{eff}}$ prediction with the proposed model, but it didn't work. The possible reason is that there is no accurate and deterministic relationship between the low-precision neutron flux distribution data and the system eigen-value parameter k_{eff}. For instance, $k_{\mathrm{eff}} = 1$ can correspond to a variety of operating power and neutron flux distributions. On the other hand, k_{eff} is a system-level eigen-value parameter (a scalar), not a distribution data. The UNet model is good at the treatment of distributed data rather than scalar value regression prediction task. A different network architecture and the use of more physical parameters (e.g., neutron scatter/absorption/fission cross section data of the system materials, temperature, boron concentration and more) as inputs are needed for accurate k_{eff} prediction.

In dynamic (time-dependent) neutronics simulation scenario, as the nuclear fission reaction proceeds, the reduction of fissile nuclide (^{235}U), the conversion of fissile nuclide (^{238}U to ^{239}Pu), and the accumulation of various types of intermediate-mass fission (e.g., ^{135}Xe) products will lead to changes in the nuclide composition in the fuel assembly, affecting the neutron reaction properties (e.g., absorption, scattering) and increasing difficulty to the DL model prediction. The burnup level used in this study was relatively small ($0 \sim 1.496$ MWd/kgIHM). The neutron flux spectrum between fresh and depleted assembly with maximum burnup level is shown in Fig. 9. The neutron flux spectrum has differences in the low-energy part (<0.001 eV) and is almost the same in the rest part. It should be noted that the proposed model may not give reliable predictions for burned fuel beyond the burnup range specified in this study, as the burned fuel exhibits significant differences in its flux spectrum from that of fresh fuel. This is a shortcoming of the proposed method. Nevertheless, the present method can also be used to accelerate neutron flux and pin power data calculations for fresh fuel and depleted assemblies with low burnup levels, providing a reference for improving the computational efficiency.

Another limitation of the proposed method lies in the requirement for a large amount of MC simulation data needs as training dataset which must be generated using MC simulations. Although the model's prediction time is fast, the training dataset preparation process is very time-consuming. Moreover, the scale, diversity and quality of the dataset determine the upper bound performance of the DL model. This is a common challenge in almost all DL-based surrogate modeling, particularly in scientific computing and engineering domains. More advanced computational frameworks and improved techniques are urgently needed for development. Collaborative efforts between the artificial intelligence and reactor physics communities will be essential to drive continued progress in high-efficiency, high-fidelity simulation techniques.

4. Conclusion

This study presents a dual-domain input UNet model for enhancing MC neutronics simulation precision. The open-source MC code OpenMC was used to simulate 2500 assembly-level low- and high-precision pin power, total and multi-group neutron flux distribution data with different cell parameters and burnup steps, producing paired dataset for model training and evaluation.

A comprehensive investigation was conducted to analyze model performance through multiple experiments: training dynamics, error analysis, loss function configurations, input data types, and training sample scales. The results show that: 1) the proposed method can be well trained, achieves stable convergence behavior, and accurately predicts the high-precision pin power, total and multi-group neutron flux distribution; 2) the hybrid loss function outperforms the single loss function, with optimal model performance observed when the weight coefficient α is 0.2 in the experiments; 3) the dual-domain data input strategy which integrates spatial and frequency-domain features, consistently outperforms single-domain input methods, highlighting the benefit of complementary feature representations.

Further studies are planned to explore the precision improvement method of 3D neutron flux distribution under axial parameter variations and develop a hybrid MC-DL framework for time-dependent pin power and neutron flux prediction, incorporating thermo-hydrodynamic coupling effects and reactivity transients, thereby advancing the applicability of DL techniques in dynamic reactor physics simulations.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

Data will be made available on request.

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