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Quantum Circuit Learning for Uncertainty Quantification of RELAP5 Code Analysis of ROSA/LSTF Small Break LOCA Tests

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Abstract. To reduce the computational demand in the best estimate plus uncertainty (BEPU) analysis, an accurate and inexpensive machine learning model is expected to be used to replace the high-fidelity RELAP5 code for rapid determination of the uncertainties on the figure of merit of interest. One of the problems associated with the application of a machine learning is overlearning. Quantum circuit learning is the quantum analogue of classical deep learning, which is expected to be less prone to overlearning because the optimized parameters are bound by unitary transformations in the quantum circuit. In this paper, quantum circuit learning is applied to the BEPU analysis of the fuel peak cladding temperature (PCT) for a small-break LOCA scenario in PWRs. The parameterized quantum circuit is trained using a small number of the RELAP5 analysis results and the prediction accuracy of the 95th percentile value of the PCTs is investigated. By optimizing the multipliers of the measured basis, the 95th percentile value of the PCTs predicted by the quantum circuit learning resulted in better accuracy and smaller variability than order statistics and linear quadratic regressions.

1 Introduction

In recent years, the best estimate plus uncertainty (BEPU) methodology [1] has been improved to better deal with loss of coolant accident (LOCA) analysis for nuclear power plants. However, in this method, the necessary high-fidelity code, such as the RELAP5 code [2] is computationally expensive. Therefore, it takes too long to perform the BEPU analysis, which limits its usefulness in nuclear safety activities such as sensitivity analysis, optimization, and other analyses. To reduce the computational demand in the BEPU analysis, an accurate and inexpensive machine learning model is expected to be used to replace the RELAP5 code for rapid determination of the uncertainties on the figure of merit of interest.

One of the problems associated with the application of a machine learning model is overlearning. To have confidence in the model prediction, it is crucial to assess the generalized performance of the machine learning model. In general, overlearning is caused by the large degree of freedom of the model and the small amount of training data. A simple regression model with a small degree of freedom can suppress overlearning, but a very simple

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model may result in inaccurate regression models. On the other hand, overlearning can be suppressed by increasing the number of training data, but many calculations using the high-fidelity code are required to construct a machine learning model. To apply a machine learning model to BEPU analysis, it is necessary to construct an appropriate machine learning model according to the complexity of the analysis target and the number of available training data.

Quantum circuit learning [3] is an algorithm using a parameterized quantum circuit as a machine learning model. It is a hybrid algorithm which consists of a part that runs on a quantum computer and a part that runs on a classical computer; in particular, it is expected to be able to run on an NISQ (Noisy Intermediate-Scale Quantum) computer. The NISQ quantum computer is a small-scale quantum computer of 50 to 100 qubits in size, including noise, and it is expected to be available within a few years to a decade. In quantum circuit learning, the structure of the parameterized quantum circuit is fixed to be executable on real hardware, and the parameters are tuned on a classical computer. Quantum circuit learning is anticipated to have the ability to suppress overlearning, because the quantum circuit is constructed using only unitary transformations which are expected to function as regularization. On the other hand, verification is needed of the computational speed and accuracy.

In a previous study by the author and Murase [4], the BEPU methodology was applied to the analysis of the LSTF small break LOCA tests with steam generator (SG) intentional depressurization as an accident management procedure [5]. The RELAP5/MOD3 code was used as the thermal hydraulic code and 1024 random calculations were conducted to get the 95th percentile values of the peak cladding temperature (PCT). Furthermore, in a later study by the author [6], a machine learning model of the uncertainty analysis of PCTs was generated using a small number of the RELAP5 analysis results as a training data set. The accuracy of uncertainty quantification of the PCTs predicted by the machine learning model based on the second order polynomial regression was investigated. The 95th percentile values predicted by the machine learning model had a smaller statistical fluctuation than the order the statistics [7, 8].

In this study, a parameterized quantum circuit was defined using Qulacs [9] and a prediction model for the uncertainty analysis of PCTs was constructed using a small number of the RELAP5 calculations as a training data set. The accuracy of the 95th percentile values predicted by quantum circuit learning was evaluated by comparing them with the results of the RELAP5 analysis, the order statistics, and the second order linear regression.

2 Uncertainty analysis by RELAP5 code

2.1 ROSA/LSTF small break LOCA tests

In a previous study by the author and Murase [4], experimental analyses using the RELAP5 code were carried out for the ROSA/LSTF small break LOCA tests with intentional SG secondary-side depressurizations [5]. Figure 1 shows a schematic of the ROSA/LSTF [5]. The LSTF was a 1/48 volumetrically-scaled, full-height, full-pressure model of a Westinghouse-type 4-loop PWR. The four primary loops of the reference PWR were represented by two equal-volume (2/48 scale) loops called Loop-A and Loop-B.

Figure 2 shows the measured [5] and predicted [4] rod surface temperatures of the SB-CL-32 test. The break position for the test was the cold leg of the loop without the pressurizer (Loop-B). The break size was 1.0% of the cold leg cross-sectional area which was equivalent

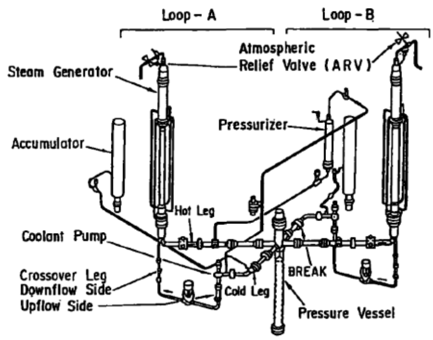


Fig. 1. Schematic of ROSA/LSTF [5].

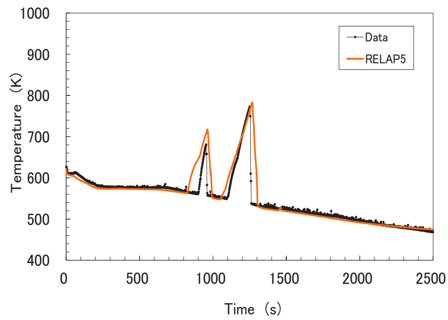


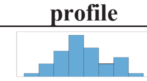
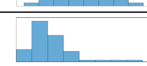
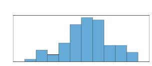
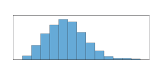
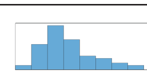
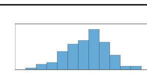
Fig. 2. Cladding temperatures of SB-CL-32 [4, 5].

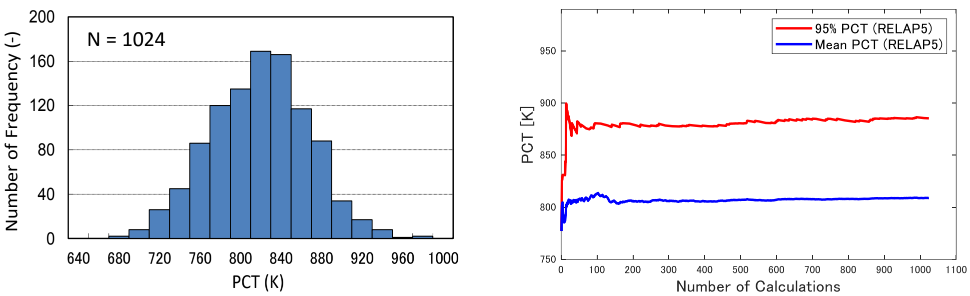
to 3 inch break for the 4-loop PWR. The SG secondary-side depressurization was initiated with the cooling rate of 200 K/h using all the SGs of the loops at 600 s after the break.

2.2 Uncertainty analysis of peak cladding temperature

Based on the BEPU methodology [1], uncertainty quantification for the analysis of the PCT was performed by the input uncertainty propagation analyses [4]. In previous studies by the author and coworkers [10], the phenomena identification and ranking table (PIRT) was developed and the RELAP5 analysis models were identified that were related to the important phenomena extracted by the PIRT. Furthermore, the uncertainties of the RELAP5 analysis models were quantified by fitting the relevant experimental data from separate effects tests. Table 1 lists the uncertainty ranges and distribution profiles of the input uncertainty parameters used in this study.

Table 1. Input uncertainty parameters.

Important phenomena	Associated RELAP5 model	Uncertainty parameter	Min	Max	Distribution profile
Uncovered core heat transfer	Dittus-Boelter correlation	Heat transfer coefficient multiplier	0.58	1.88	
Interfacial friction in the core	Drift flux model, EPRI correlation	Interfacial friction coefficient multiplier	0.13	3.00	
Condensation heat transfer in U-tubes (laminar)	Nusselt correlation	Condensation heat transfer coefficient multiplier	0.56	1.44	
Condensation heat transfer in U-tubes (turbulent)	Shah correlation	Condensation heat transfer coefficient multiplier	0.64	1.66	
CCFL at inlet of U-tubes	CCFL model	CCFL constant	0.70	0.80	Uniform
Horizontal stratification in cold legs	Taitel-Dukler model	Horizontally stratified flow criterion multiplier	0.20	4.63	
Interfacial friction in downcomer	Drift flux model, Kataoka-Ishii correlation	Interfacial friction coefficient multiplier	0.58	1.60	



(a) Histograms (b) Convergence processes

Fig. 3. Uncertainty of PCT [4].

The input uncertainty propagation analyses for the experimental analysis were performed with the variance of each parameter listed in Table 1 by using a simple random sampling method. In this study, 1024 random calculations were conducted to get the 95th percentile values of the PCT. Figure 3(a) shows the histogram of the PCTs. Figure 3(b) shows the convergence processes of the 95th percentile values and the mean values of the RELAP5 analyses during the 1024 Monte Carlo sampling histories.

3 Application of quantum circuit learning

In order to reduce the computational demand for the thermal hydraulic system calculations in the BEPU analysis, a machine learning model is expected to be used for rapid determination of the uncertainties on the system figure of merit of interest. One of the problems associated with the application of a machine learning is overlearning. Quantum circuit learning is the quantum analogue of classical deep learning, which is expected to be less prone to overlearning because the optimized parameters are restricted by the unitary transformation.

3.1 Quantum circuit learning

Figure 4 shows a conceptual diagram of quantum circuit learning. Quantum circuit learning [3] is an algorithm using a parameterized quantum circuits as a machine learning model. The algorithm optimizes the parameters to minimize the difference between the output from the parameterized quantum circuit and the training data. It is a hybrid algorithm having a part that runs on a quantum computer and a part that runs on a classical computer; in particular, it is expected to be able to run on an NISQ computer, which is a small-scale quantum computer that is expected to be available within a decade. In quantum circuit learning, the structure of the parameterized quantum circuit is executable on real hardware, and the parameters are tuned on a classical computer. Quantum circuit learning is expected to have the ability to suppress overlearning, because the quantum circuit is constructed using only unitary transformations which are anticipated to function as regularization. On the other hand, verification is needed of the computational speed and accuracy.

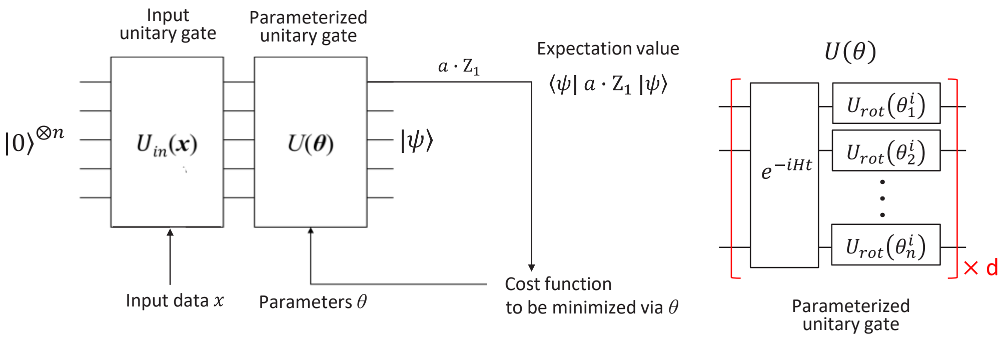


Fig. 4. Framework of quantum circuit learning.

In this study, the quantum circuit model is constructed according to the literature [11] as described briefly below.

The input unitary gate $U_{in}(x)$ encodes the input data x by using rotation gates $R_j^X(\theta) = e^{i\theta X_j/2}$ and $R_j^Z(\theta) = e^{i\theta Z_j/2}$ as follows:

$$U_{in}(x) = \prod_j R_j^Z(cos^{-1}x^2)\, R_j^Y(sin^{-1}x) \tag{1}$$
$$R_j^Y(\theta) = e^{i\theta Y_j/2} \tag{2}$$
$$R_j^Z(\theta) = e^{i\theta Z_j/2} \tag{3}$$

The parameterized unitary gate $U(\theta)$ is defined by layering (i = 1,...,d) compositions of the time evolution operator U_{rand} and the rotation gate $U_{rot}(\theta_j^i)$ acting on the j-th (j = 1,...,n) qubit. d is the depth of the unitary gate $U(\theta)$. $U_{rand} = e^{-iHt}$ is the time evolution operator of the transverse field Ising model, which increases the complexity of the quantum circuit. $U_{rot}(\theta_j^i)$ is consisted of rotation gates $R_j^X(\theta) = e^{i\theta X_j/2}$ and $R_j^Z(\theta) = e^{i\theta Z_j/2}$, whose rotation prameters $\{\theta_j^i\}$ are optimized.

$$U(\{\theta_j^i\}) = \prod_{i=1}^{d}\left(\left(\prod_{j=1}^{n} U_{rot}(\theta_j^i)\right)\cdot U_{rand}\right) \tag{4}$$

$$U_{rand} = e^{-iHt} \tag{5}$$
$$H = \sum_{j=1}^{N} a_j X_j + \sum_{j=1}^{N}\sum_{k=1}^{j-1} J_{jk} Z_j Z_k \tag{6}$$

$$U_{rot}(\theta_j^i) = R_j^X(\theta_{j1}^i)\, R_j^Z(\theta_{j2}^i)\, R_j^X(\theta_{j3}^i) \tag{7}$$
$$R_j^X(\theta) = e^{i\theta X_j/2} \tag{8}$$
$$R_j^Z(\theta) = e^{i\theta Z_j/2} \tag{9}$$

Quantum circuit learning is performed by adjusting the rotation angles $\{\theta_j^i\}$ of the unitary gate $U(\theta)$ and the multiplier a of Z-basis which widens the value range of the computational basis. In this paper, the multiplier a is treated as a hyperparameter. The details of the algorithm are provided below.

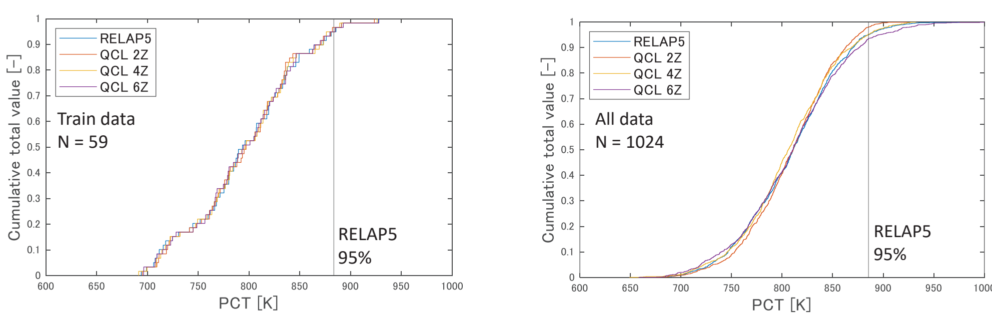
1. The initial state $|0\rangle^{\otimes n}$ is converted to an input state $|\psi_{in}(x)\rangle$ by the input unitary gate $U_{in}(x)$ which encodes the input data x.
2. The input state is converted to an output state $|\psi\rangle = |\psi(x, \theta)\rangle$ by the parameterized unitary gate $U(\theta)$.
3. The model output y_{out} is defined as the expected value $\langle\psi|a \cdot Z_1|\psi\rangle$ of the output state $|\psi\rangle$ measured by the Pauli Z operator in the first qubit multiplied by the multiplier a.
4. The loss function $\mathrm{L} = \mathrm{L}(\theta)$ is defined as the least-squares error between the output $\{y_{out}\}$ and the true value $\{y\}$.
5. The rotation angles $\theta = \{\theta_j^i\}$ are optimized so that the lost function $\mathrm{L}(\theta)$ is minimized.

In this model, the depth d of layers of the parameterized unitary gate $U(\theta)$ is another hyperparameter. The depth d should be set to a large value depending on the complexity of the modeling target.

3.2 Uncertainty analysis by quantum circuit learning

In this study, a 7-qubit quantum circuit was defined using a quantum simulator Qulacs [9] and a prediction model for the uncertainty analysis of PCTs was constructed using 59 randomly selected samples of RELAP5 calculations as a training data set. In this paper, the depth of the parameterized unitary gate was set to 9.

Figure 5 shows the cumulative distribution functions of the PCTs evaluated by quantum circuit learning for the training data (59 samples) and for all data (1024 samples), compared to the RELAP5 calculation results. The cumulative distribution functions of the PCTs for the training data are in good agreement with the RELAP5 calculations for each multiplier, where the multipliers are 2, 4, and 6, which expand the value range of the computational basis (Z basis) to be measured. On the other hand, for all data, the cumulative distribution function agrees well with the RELAP5 calculation only when the multiplier is 4.



(a) Training data (b) All data

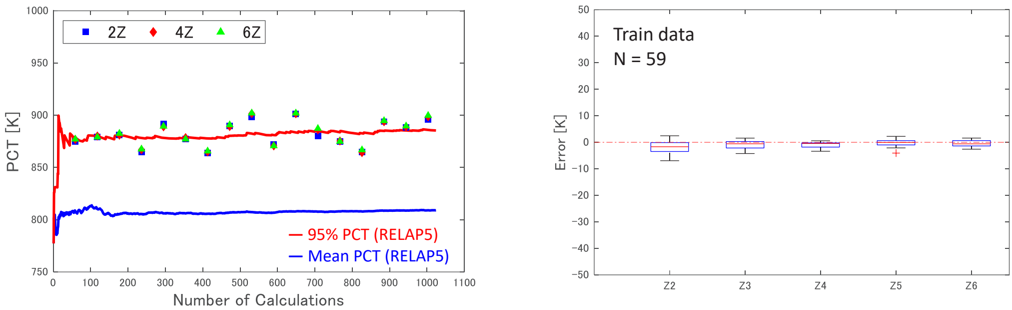
Fig. 5. Cumulative distribution functions of PCT.

Figures 6 and 7 show the predicted results of the 95th percentile values for the training data and for all data, respectively, by the quantum circuit models constructed using 59 consecutive samples (17 cases in total) of the RELAP5 calculations as training data.

Figures 6(a) and 7(a) plot the predicted 95th percentile values for the training data and for all data, respectively, with the Z-basis multipliers of 2, 4, and 6, along with the convergence process of the 95th percentile values of the RELAP5 calculations. The predicted 95th percentile values (17 cases in total) for the training data are consistent across the all Z-basis multipliers. On the other hand, the predicted 95th percentile values (17 cases in total) for all data are different depending on the Z-basis multipliers.

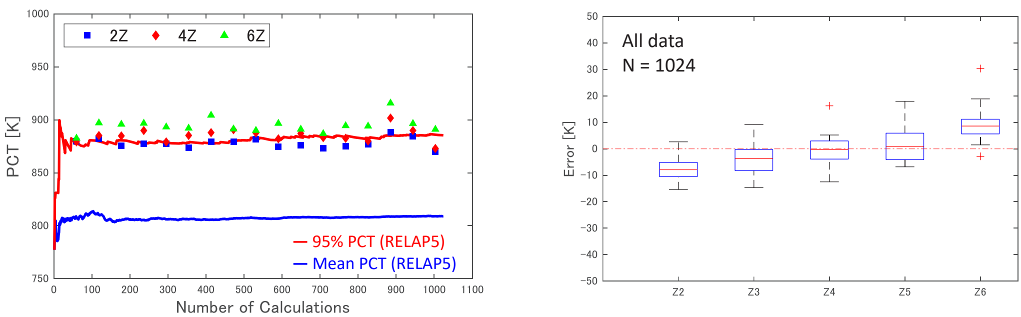
Figures 6(b) and 7(b) are boxplots of the prediction errors (17 cases in total) by quantum circuit learning for the training data and for all data, respectively, with the Z-basis multipliers of 2, 3, 4, 5, and 6. For the training data, the prediction errors are almost zero for all Z-basis multipliers. On the other hand, for all data, the prediction error is the smallest when the Z-basis multiplier is 4.

From the above results, it is confirmed that an appropriate selection and use of the Z-basis multiplier defines a parametrized quantum circuit with good prediction accuracy of the 95th percentile values of PCTs calculated by the RELAP5 code for all data. The important point to note is that it is necessary to use the training data to determine the appropriate Z-basis multipliers.



(a) Predicted 95th percentile values (b) Prediction erros

Fig. 6. Prediction of 95th percentile values of PCT for training data.



(a) Predicted 95th percentile values (b) Prediction erros

Fig. 7. Prediction of 95th percentile values of PCT for all data.

3.3 Optimization of Z-basis multipliers

This study sought to investigate the effectiveness of a cross validation technique to optimize the Z-basis multipliers, that is to estimate the prediction accuracy for the 95th percentile values of PCTs for all data using only the training data set.

Figure 8 presents a conceptual diagram of k-fold cross validation. First, the training data are partitioned into k-equally sized segments. Next, k iterations are performed for training and validation such that within each iteration, a fold of the data is held out for validation while the remaining k-1 folds are used for training. In this way, in cross validation, data are each separately used as validation data and training data, so the evaluation is not biased toward specific data. Therefore, the evaluation is considered to have generalization performance for data other than the training data.

Figure 9 summarizes the evaluated results of the 95th percentile values for the training data by the cross validations of the quantum circuit models constructed using 59 consecutive samples (17 cases in total) of the RELAP5 calculations as training data. As seen in Figure 9(a), the evaluated results of the 95th percentile values (17 cases in total) differ depending on the Z-basis multipliers. As shown in Figure 9(b), the prediction error of the 95th percentile values is the smallest when the Z-basis multiplier is 4.

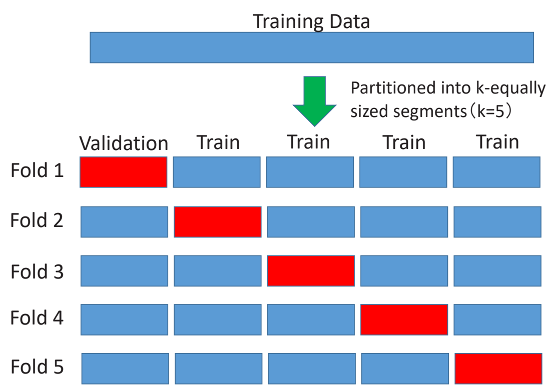
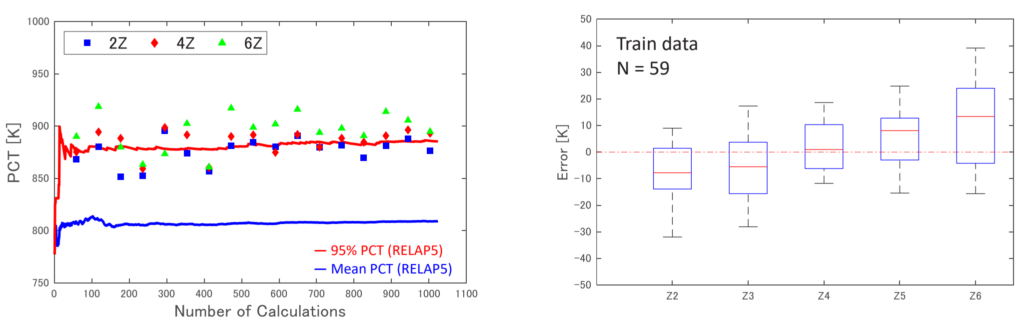


Fig. 8. k-flold cross validation.

Therefore, the Z-basis multipliers with the minimum error for the predicted 95th percentile values by the quantum circuit learning for all the data can be estimated by cross validation using the training data set. It is confirmed that using the Z-basis multipliers with which the 95th percentile PCT error is estimated to be minimized by cross validation, the 95th percentile value predicted by the quantum circuit learning agrees well with the 95th percentile PCT by the RELAP5 analysis.

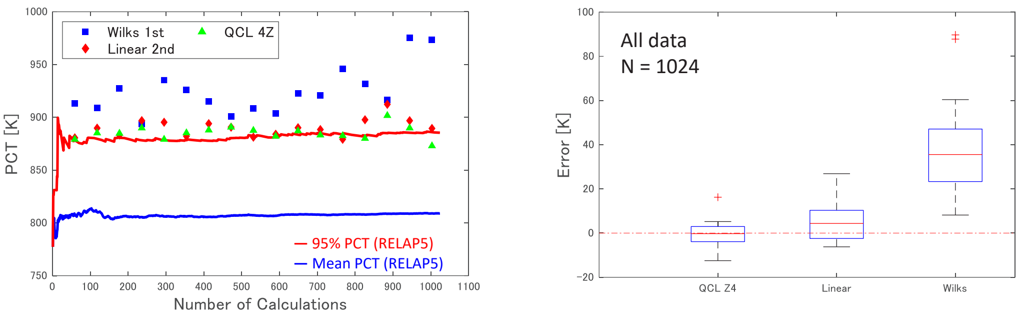


(a) Predicted 95th percentile values (b) Prediction erros

Fig. 9. Prediction of 95th percentile values of PCT by cross validation.

4 Comparison with order statistics and linear regressions

In order to find the uncertainty range with a limited number of runs, one practical approach is to get the 95%/95% tolerance limit values by using Wilks formula [7, 8]. Wilks formula is derived based on order statistics. Order statistics is a method of assessing uncertainty by determining the number of samples (i.e. number of analysis cases) required to obtain an evaluation value for a given confidence level based on statistical theory. The number of samples required for the 95th percentile value to be placed at the first in order at the 95% confidence level is evaluated as 59 samples.



(a) Predicted 95th percentile values (b) Prediction erros

Fig. 10. Comparison of predicted 95th percentile values of PCT for all data.

Figure 10 compares the 95th percentile values of PCTs for all data by the Wilks formula, the second order polynomial regression, and the quantum circuit model with Z-basis multiplier of 4, which were evaluated using 59 consecutive samples (17 cases in total) of RELAP5 calculations as training data. It is confirmed that the predictions by quantum circuit learning with the optimized Z-basis multiplier show better accuracy and smaller variation than the evaluation by order statistics and linear quadratic regression.

5 Conclusions

In this study, quantum circuit learning was applied to the RELAP5 code uncertainty analysis of the PCT for the ROSA/LSTF small break LOCA tests. A parameterized quantum circuit was defined and a prediction model for the uncertainty quantification of PCT was constructed using a small number of the RELAP5 calculations as a training data set. The accuracy of the 95th percentile values predicted by quantum circuit learning was evaluated by comparing them with the results of the RELAP5 analysis, the order statistics method, and the second order linear regression.

(1) A quantum circuit model with an appropriately selected Z-basis multiplier provided good prediction accuracy for the 95th percentile value of the PCTs calculated by the RELAP5 code.
(2) The cross validation using the training data set could estimate the Z-basis multipliers of the quantum circuit model with the minimum error for the predicted 95th percentile values.

(3) The 95th percentile value predicted by the quantum circuit model with the optimized Z-basis multiplier provided better accuracy and smaller variation than the evaluation by order statistics and linear quadratic regression.

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References

1. B. Boyack, R. Duffey, P. Griffith, G. Lellouche, S. Levy, U. Rohatgi, G. Wilson, W. Wulff, N. Zuber, *Quantifying Reactor Safety Margins: Application of Code Scaling, Applicability, and Uncertainty Evaluation Methodology to a Large-Break Loss-of-Coolant Accident*, NUREG/CR-5249 (1989)
2. The RELAP5 Code Development Team, *RELAP5/MOD3 Code Manual*, NUREG/CR-5535 (1995)
3. K. Mitarai, M. Negori, M. Kitagawa, K. Fujii, *Quantum circuit learning*, PHYSICAL REVIEW A **98**, 032309 (2018)
4. I. Kinoshita, M. Murase, *RELAP5 Code Analysis of LSTF Small Break LOCA Tests with Steam Generator Intentional Depressurization and Its Uncertainty Quantification by Monte-Carlo Method and Wilks' Formula Approach*, Proceedings of the ASME 2016 International Mechanical Engineering Congress & Exposition (IMECE2016), IMECE2016-66638, Phoenix, AZ, November 11-17, (2016)
5. H. Asaka, Y. Anoda, Y. Kukita, I. Ohtsu, *Secondary-Side Depressurization during PWR Cold-Leg Small Break LOCAs Based on ROSA-V/LSTF Experiments and Analyses*, Journal of Nuclear Science and Technology, **35**(12), pp.905-915 (1998)
6. I. Kinoshita, *Application of Surrogate Model for Uncertainty Quantification of RELAP5 Code Analysis of LSTF Small Break LOCA Tests*, Proceedings of 27th International Conference on Nuclear Engineering (ICONE27), ICONE27-2428, Ibaraki, Japan, May 19-24 (2019)
7. S.S. Wilks, *Statistical prediction with special reference to the problem of tolerance limit*, Annals of Mathematical Statistics, **13**, pp.400-409 (1942)
8. A. Guba, M. Makai, P. Lenard, *Statistical aspects of best estimate method-I*, Reliability Engineering and System Safety, **80**, pp.217-232 (2003)
9. Y. Suzuki, et al., *Qulacs: a fast and versatile quantum circuit simulator for research purpose*, arXiv:2011.13524v4 (2021)
10. M.J. Griffiths, J.P. Schlegel, T. Hibiki, M. Ishii, I. Kinoshita, Y. Yoshida, *Phenomena identification and ranking table for thermal-hydraulic phenomena during a small-break LOCA with loss of high pressure injection*, Progress of Nuclear Energy, **73**, pp.51-63 (2014)
11. QunaSys Inc., *Welcome to Quantum Native Dojo!*, https://dojo.qulacs.org/ja/latest/index.html (2024) (in Japanese)