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INTRODUCTION

Quantification of nuclear power plant safety risk requires a systematic and yet practical approach to identification of accident scenarios, assessment of their likelihood and consequences. Instrumental to this goal is risk-informed safety margin characterization (RISMC) framework, whose realization requires computationally robust and affordable methods for sufficiently accurate simulation of complex multi-dimensional physical phenomena, such as turbulent and multi-phase flow. The CFD-like codes with 3D simulation capability and full treatment of momentum transport terms (e.g., GOTHIC [1]) ensure computational efficiency using coarse mesh size and the sub-grid phenomena in the boundary layer that can be captured by adequate constitutive correlations (e.g., wall functions and turbulence models). However, the error sources and user effects on the selection of mesh size and models lead to unpredictable simulation error, while rich High-Fidelity (HF) data from experiments and numerical simulation using validated code or Direct Numerical Simulation (DNS) are not fully explored. It would be useful to have a "smart" data-driven multi-scale framework in which the low-resolution models can be "taught" to emulate high-resolution models.

The objective of this work is to develop and evaluate a physical-based data-driven mesh-model optimization approach (Optimized Mesh/Model Information System, OMIS) to estimate the simulation error and give advice on the optimized selection of coarse mesh size and models for Low-Fidelity (LF) simulation (e.g., System Thermal Hydraulic, CFD-like or CGCFD) to achieve accuracy comparable to that of HF models. This approach takes advantages of computational efficiency of coarse-mesh simulation and application of Machine Learning (ML) algorithms.

ERROR ANALYSIS OF COMPUTATIONAL CODE

Considering the drawbacks of Lumped-Parameter (LP) codes and CFD codes, some CFD-like codes, such as GOTHIC, have natural advantages: (1) Coarse mesh and 3D capability ensures computational efficiency and the sufficient local information that can be captured; (2) Sub-grid phenomena in the boundary layer can be taken into consideration using adequate boundary-layer empirical correlations (i.e., wall functions). GOTHIC is selected as the computational code for the development of the OMIS approach because GOTHIC can be used in both STH (LP or 1D model, no turbulence effects) and CFD-like (multi-dimensional with full treatment of momentum transport terms and turbulence models) modes.

There are two main error sources in STH or CFD-like codes. The first one is the model error due to physical simplification and mathematical approximation on these applied models. These types of codes use boundary-layer correlations for heat, mass and momentum exchanges between the fluid and the structures, rather than attempting to model the boundary layers specifically. [1] The key local phenomena in near-wall region are friction, turbulence and heat transfer. Respective correlations are applied where characteristic lengths (determined by mesh size) are introduced as one of the model parameters. The other one is the mesh error due to the information loss of conservation equations and source terms using time and space averaging approaches, which is also determined by mesh size. Other numerical errors due to iterative convergence, algorithm selection, coding error and finite arithmetic have less influence on the modeling and simulation compared to model error and mesh error.

Considering the tight connection with mesh size, model error and mesh error cannot be estimated separately. The finite mesh approach could fail in not capturing the expected local behaviors of the fluids, while fine mesh may introduce a violation of the Courant limit issue or an improper extending of boundary-layer empirical correlations. These factors make the selection of mesh size and model an important but tricky task in the modeling and simulation.

REVIEW OF APPLICATION OF MACHINE LEARNING TO THERMAL-HYDRAULIC SIMULATION

Despite decades of work, the difficulties in performing validation and verification of STH codes and dealing with the uncertainty/error sources still exist. The development of nuclear reactor thermal-hydraulics lags behind the improvements in knowledge and computer capability. In NURETH-15, Dinh [2] proposed perspectives on the nuclear reactor thermal-hydraulics, and envisioned that "in the future, the complex and varied issues of nuclear reactor thermal-hydraulic processes could be addressed effectively and efficiently by developing and implementing a data-driven framework for modeling and simulation that brings together and allows for all relevant data and knowledge to be utilized together to enable synergistically predictive tools and processes for nuclear thermal-hydraulics." The concept of a data-driven modeling and simulation framework enables the simulation code applying pattern recognition and statistical analysis to obtain closure information directly from the relevant database. For conditions where applicable data are absent, the information can be estimated and predicted based on the near-by conditions included in the database. At the core of this framework are methods and tools for Total Data-Model Integration (TDMI) that bring together data, models and simulations to effectively support decision-making.

There have already been several efforts to apply Machine Learning (ML) algorithms on fluid dynamics since the beginning of this century, which were mainly focused on the development of data-driven turbulence closures in order to deal with the issues from CFD model form uncertainty and lack of knowledge. Meanwhile, Hanna [3] investigated the feasibility of a Coarse Grid (CG) CFD approach using ML algorithms to produce a surrogate model that predicts the CG-CFD local errors to enable correction of the CG results. This work focused on the correction of discretization error considering the model errors that may be introduced in CG-CFD applications. All these data-driven approaches are not designed to predict the thermal-hydraulic simulation error using STH or CFD-like codes. Model error and numerical error are each analyzed individually with the other fixed, the logic of which is impractical to these codes where the model error and mesh error cannot estimated separately. Chang [4] introduced a classification of machine learning frameworks for thermal fluid simulation including five types. Current efforts mainly belong to Type I and II ML. Type II ML is focused on reducing the uncertainty from closure laws to conservation equations. The OMIS approach proposed in this paper can be considered as a kind of Type II.

ML algorithms are applied to realize the data-driven concept by using computational methods to "learn" information directly from data without assuming a predetermined equation as a model. These algorithms adaptively improve their performance as the number of samples available for learning increases. The goal is to find natural patterns in data that generate insight and help make better decisions and predictions. Feedforward Neural Networks (FNNs) work well for high dimensionality problems with large datasets while little knowledge about the underlying process or suitable physical features exist. A FNN is an information processing paradigm that is inspired by the way biological nervous systems, such as the brain, process information. The key element of this paradigm is the novel structure of the information processing system. It is composed of a large number of highly interconnected processing elements (neurons) working in unison to solve specific problems in parallel. As in nature, the connections between elements largely determine the network function. Typically, NNs are adjusted and trained so that a particular input leads to a specific target output. Currently, FNNs are identified as the efficient ML algorithm for OMIS approach.

METHODOLOGY

The central idea of the OMIS approach is shown in Fig. 1. The simulation error (ε) for the physics of interest using these coarse-mesh STH or CFD-like codes integrates the model error (ε_{model}), mesh error (ε_{mesh}) and other numerical errors. Considering that the former two error sources have heavier weights, the ideal way is to find the relationship between ε and ε_{model}, ε_{mesh}. However, these two error sources cannot be quantified separately because of the tight connections with mesh size. The key to the OMIS approach is to develop a surrogate model to identify the relationship between ε and local Physical Features (PFs) which integrate the physical information, model information and effect of mesh size. Once the function ε=f(PFs) is developed, the simulation error for new condition with the specific mesh and model is supposed to be predictable. The mesh size and model with least simulation error are identified as the optimized mesh size and model for the specific physical system, which means that they are the "best" choice for the simulation for this condition.

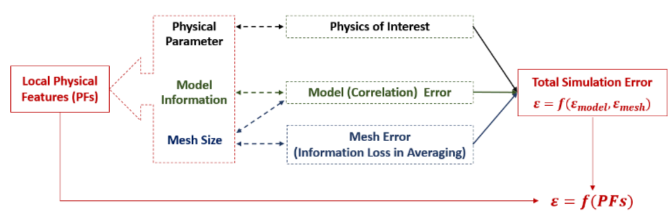


Fig. 1. Central Idea of the OMIS Approach

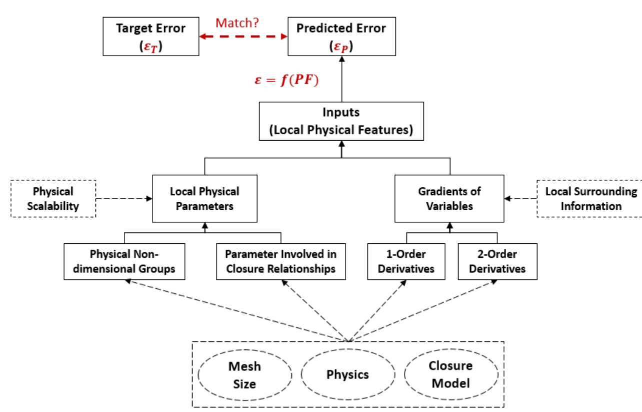


Fig. 2. Structure of OMIS Model: Input and Output

The basic hypotheses for the OMIS methodology are: (1) The length scale of the physics of interest is large enough to be captured by coarse-mesh modeling. (2) The

STH or CFD-like code is able to capture the basic physical behaviors of the system of interest (3) Model error and mesh error are the main error sources and must be quantified jointly (they cannot usefully be quantified separately). (4) HF data are qualified and sufficient for ML to learn from and find the intrinsic knowledge of the physics. (5) The simulation error can be represented as a function of key PFs that integrate the physical information of the physical system, model and the effect of mesh size.

The structure of the OMIS model is displayed in Fig. 2. The identification of PFs takes both of local physics and scalability into consideration, including mainly the gradients of local variables and local physical parameters that are able to represent the local physical behaviors or be applied in closure relationships for the boundary layer. The central-difference formulas are applied to calculate the derivatives of variables. The gradients of local variables imply the local surrounding information that represents the local physical patterns, as displayed in Fig. 3. The local information obtained from the training dataset can be used to "teach" the prediction of new conditions but with similar local physical patterns. Another part of PFs is the local parameters that are able to represent the local physical behaviors. These parameters representing the local physical behaviors are also supposed to provide the scalability. A third part of PFs are the parameters that are used or involved in the local closure correlations for boundary layer simulation. These parameters contain much information of length scale, model parameter and local geometry.

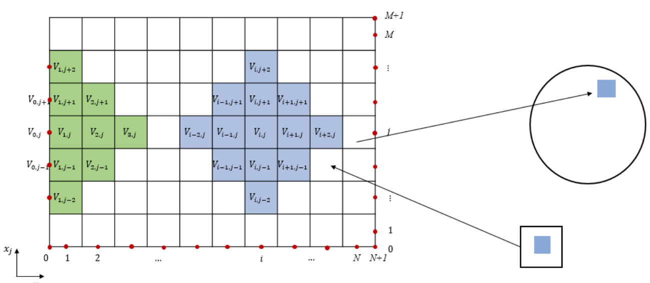


Fig. 3. Arrangement of Nodes in 2D Problems

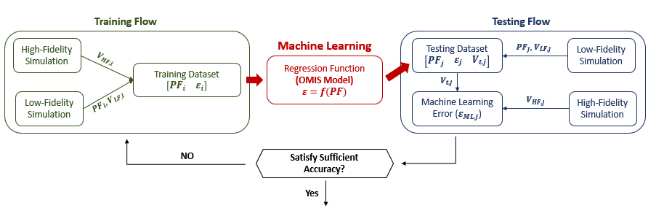


Fig. 4. Schematic of OMIS Approach: Training and Testing

The information flow of the OMIS approach is described in Fig. 4. In training part, LF simulations with different discontinuous global features are performed and then compared with HF data. The local errors (ε_i) of variables between mapped HF data ($V_{HF,i}$) and LF simulations ($V_{LF,i}$) are calculated and collected to obtain the error training database. The PF values (PF_i) of training part are obtained using LF simulation results. The regression error function, defined as the OMIS model (ε=f(PFs)), is obtained based on the training database by applying ML algorithms. Then by inserting the new PF values (PF_j) of testing part into the OMIS model, the respective errors (ε_j) can be predicted to modify the LF simulation results ($V_{LF,j}$). Then the modified variable values ($V_{t,j}$)are compared with the ones from HF data ($V_{HF,j}$). The predictive capability of local OMIS model is tested via validation metrics (Machine Learning Error, $\varepsilon_{ML,j}$) to check whether the prediction satisfies the accuracy requirement. The determination of sufficient accuracy is based on simulation purpose and knowledge limit on true physics.

The uncertainty exists in the OMIS prediction on the simulation error no matter which ML algorithm is applied. The validation metric, Mean Squared Error (MSE) is identified and applied to evaluate the predictive capability for the error estimation of the applied ML algorithm. The uncertainty from the randomness of initial weights and biases in FNN is reduced by running FNN with fixed number of layers and neurons for many times and calculating the MSE of prediction mean. m is the running times and n is the number of data points.

$$MSE_{mean\ of\ prediction} = \frac{1}{n}\sum\left(\boldsymbol{u_{HF}} - \frac{1}{m}\sum_{i}^{m}\boldsymbol{u_{predicted,i}}\right)^2 \quad (1)$$

RESULTS OF CASE STUDY

As shown in Fig. 5, an adiabatic turbulent mixing cavity with air injection on bottom of one side wall and a vent on the other side wall is used as the case study to illustrate the framework and evaluate the OMIS predictive capability on simulation error.

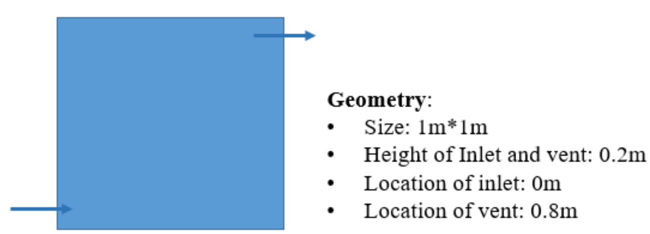


Fig. 5. Adiabatic Turbulent Mixing in a Square Cavity

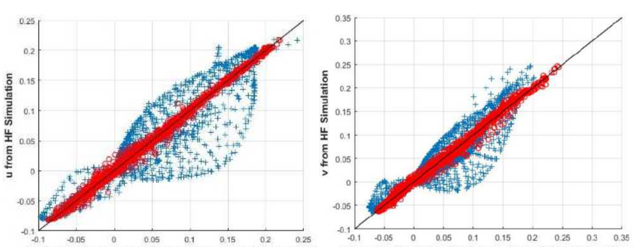
The injection Re number (Re_{inj}) is calculated based on the inlet rate and the inlet diameter as characteristic length. Four cases are simulated with different injection flow rates with Re_{inj} values as 8000, 10000, 12000, 14000. HF data and LF data were respectively obtained from the simulations of STAR CCM+ and GOTHIC. The potential local PFs selected for the case study include the 1-order and 2-order derivatives of velocities, modified local Re number containing the mesh information and the wall distance, and viscosity ratio of turbulent viscosity and air viscosity. The outputs are the velocity difference (u as vertical velocity and v as horizontal velocity) between HF data and LF data.

Four tests are developed considering the interpolation and extrapolation of the different global parameters, as shown in Table 1T. FNN with 20 neurons is used as ML algorithm for data training. The simulation errors of velocity are predicted and added on the GOTHIC results. The modified velocity in each coarse-mesh cell is then compared with the averaged value mapped from HF data.

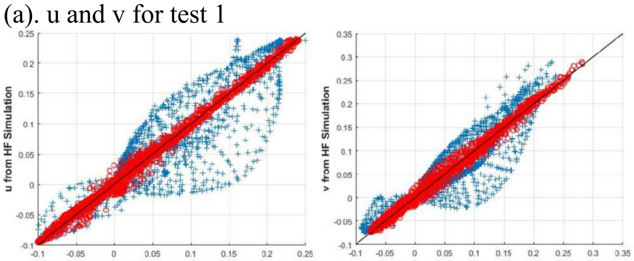
TABLE 1. Description of Tests

Test NO.		Training Case	Testing Case
1	Interpolation of Re_{inj}	Re_{inj} =8000, 1000, 14000	Re_{inj} =12000
2	Extrapolation of High Re_{inj}	Re_{inj} =8000, 1000, 12000	Re_{inj} =14000
3	Interpolation of Mesh	Mesh = 1/5, 1/10, 1/20, 1/25, 1/30	Mesh = 1/15
4	Extrapolation of Fine Mesh	Mesh = 1/5, 1/10, 1/15, 1/20, 1/25	Mesh = 1/30

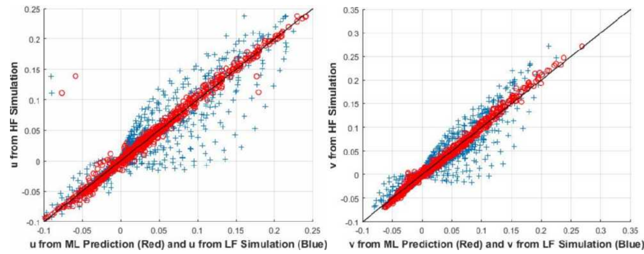
Fig. 6. Shows the comparisons between original GOTHIC results and modified values by OMIS. The vertical axis is the HF data averaged velocity from STAR CCM+. The values of predicted u and v (Red circles) were quite close to the values from HF data with small values of MSE. Blue points are the comparison between LF results and HF data. OMIS approach represents good predictive capability and scalability on estimating the local simulation error within an acceptable uncertainty even for the extrapolation of global physics.



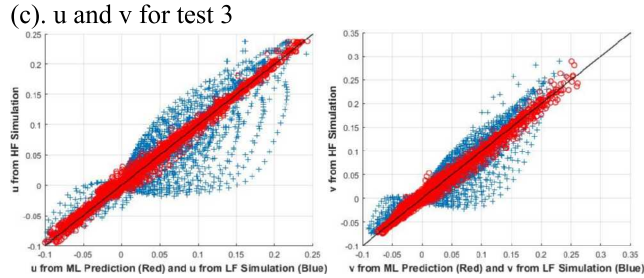
(a). u and v for test 1



(b). u and v for test 2



(c). u and v for test 3



(d). u and v for test 4

Fig. 6. Comparisons between Modified Values by OMIS (Red) and Original GOTHIC Results (Blue)

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