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Changing the World's Energy Future

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Idaho National Laboratory

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Machine Learning in Nuclear Thermal Hydraulics, Part 2: Opportunities and Perspectives

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Abstract

This paper summarizes the issues in nuclear thermal hydraulics (NTH), mainly from the three named aspects, and illustrates potential opportunities of machine learning (ML) applications in dealing with these issues. These issues are problems in simultaneously realizing computational efficiency and accuracy of system thermal-hydraulic (STH) modeling and simulation, uncertainty in the scaling analysis for the best-estimate calculations of transient and accident analysis, and difficulties in optimal data production and usage for the development and assessment of evaluation models. Due to ML uncertainty, data insufficiency, and lack of cognition about how to efficiently incorporate knowledge and data, challenges of adapting ML techniques still exist. Accordingly, several perspectives are proposed to provide insights for ML applications in solving these issues.

1. Issues

1.1. Issue #1: Efficiency vs. Accuracy

Thermal-hydraulics is the physics of fluid flow and energy transfer, as well as the interactions between fluid flow, energy, and the surrounding structures. Thermal-hydraulics in nuclear reactors is a wide-ranging subject that includes a huge number of diverse topics, which may range from one-dimensional to 3D flow fields that interact with structures that may be represented as point to 3D bodies with heat sources and/or sinks. For many of the scenarios that must be considered in nuclear reactors, important variables and phenomena change as a function of time. [1] With the rapid increase of the interest in advanced reactors, such as small modular reactors and microreactors, the nuclear thermal hydraulics (NTH) faces far bigger challenges with unfamiliar fluids and structures. Besides, their compact, elaborate, but complicated system designs make advanced-reactor designs exhibit strong 3D behaviors, which raises requirements on the efficiency and accuracy of system thermal hydraulic (STH) modeling and simulation. In past decades, several types of thermal hydraulic codes have been extensively developed, assessed, and used to support design, licensing, and safety analysis of the plants, but it is still difficult to achieve computational efficiency and accuracy simultaneously.

A significant difficulty is caused by the complexity of these multidimensional multiphase physical phenomena in transient scenarios. These phenomena occur in different nuclear power plant (NPP) components with complex geometries and structures, making it impossible to perfectly model and simulate the entire NPP thermal-hydraulic systems in all time and length scales. Different types of computational codes have been developed and used for thermal-hydraulic analysis. The first type is called lumped-parameter or system code, such as RELAP 5 and TRAC. These codes describe an NPP thermal-hydraulic system as a network of simple control volumes connected with junctions. Turbulence effects are not directly modeled, but up to a point, they can be considered using assumed flow-loss coefficients in the momentum equation. [2] When time- and geometry-averaging approaches are applied on local instantaneous two-fluid models to speed up computation, much local information is lost (including multidimensional effects); though, nowadays, some versions of these codes also have the three-dimensional capability with coarse-mesh nodalizations. Additionally, conservation equations have simplified forms in a sense that they assume physics and scale separation with highly empirical closures developed for steady-state fully-developed conditions, but being applied for transient scenarios. The second type is Computational Fluid Dynamics (CFD), which has become more commonly used to solve transport equations of fluid mechanics (continuity, momentum, and energy) using a local instantaneous formulation. These CFD codes (e.g., STAR-CCM+) consider turbulence effects using different turbulent models. STH analysis using CFD codes is computationally expensive since millions of cells might be needed, even for modeling of a single NPP component. The third type of code is a CMCFD-like code (e.g., GOTHIC) which is a compromise of the previous two types aiming at obtaining a balance between efficiency and accuracy. These codes provide a 3D-simulation capability and use a coarse mesh size with the sub-grid phenomena in boundary layer being well captured by adequate constitutive correlations (e.g., wall functions and turbulence models), which makes these codes very computationally efficient. As differentiated from standard system codes (with much loss of local information) and standard CFD codes (with huge computational cost), these codes have natural advantages for achieving sufficient accuracy for long-term multiple-component, system-level simulation.

However, two main error sources exist in the application of these coarse-mesh CFD-like codes. One is model error due to physical simplification and mathematical approximation on these applied models, correlations, and assumptions. They solve the integral form of conservation equations for mass, momentum, and energy for multicomponent, multiphase flow. Boundary-layer correlations are applied for heat, mass, and momentum exchanges between the fluid and the structures, rather than attempting to resolve the boundary layers specifically. The respective characteristic lengths of these empirical correlations are calculated by default using the local mesh size. Therefore, the mesh size greatly affects performance of the empirical correlations in the local near-wall cells and becomes a key model parameter that determines whether the correlations are being applied in appropriate ranges. Another source of error is mesh-induced error, which indicates the information loss of conservative and constitutive equations during the application of time- and space-averaging approaches. The local instantaneous partial differential equations (PDEs) for mass, momentum, and energy balance are space-averaged to obtain the finite-volume equations. Simulation results represent the averaged values of parameters over specified regions, which ignore the local gradient information. A similar concept, discretization error, is proposed from the classic Verification and Validation (V&V) point of view for solving PDEs, which assumes that, when mesh size goes to zero, the solution of PDEs converges. However, due to the correlation-based design in the simplified boundary-layer treatment, these CFD-like codes are not expected to converge when mesh size goes to zero because these empirical correlations may no longer be valid for very fine mesh.

Because both main error sources are tightly connected with local mesh size, the nodalization of control volumes determines whether the user can get a relatively good simulation result. The finite mesh/volume approach, particularly in the coarse scheme of nuclear power plant (NPP) simulations, could fail to capture the expected local behaviors of the fluids (sharp gradients of variables) due to limited resolution. On the other hand, a finer nodalization could introduce an improper extrapolation of boundary-layer empirical correlations. All these factors make the selection of mesh size and model information (model parameter and model form) an important, but tricky task in system-level thermal-hydraulic modeling and simulation using these CFD-like codes. Generally, the mesh size and models are selected based on previous simulation experience or are available in modeling guidelines derived from past benchmarking and application of the code; however, this kind of "educated guess" or engineering judgement may lead to an unknown error for the new physical conditions. Therefore, a question can be posed here: how to simultaneously realize computational efficiency and accuracy of STH modeling and simulation.

1.2. Issue #2: Scaling Uncertainty

Scaling in NTH refers to the process of assessing the similarity of phenomena that occurred and were observed in a reduced-scale test facility and the full-scale NPP application. Because it is impractical to perform experiments under prototypic conditions, the prediction of prototype-scale processes is normally made by models developed based on scaled experiments. These scaled experiments are designed by decomposing and down-scaling the full-scale applications into a series of tests that attempt to isolate individual phenomena. These are often referred to as separate-effects tests (SETs). The phrase "scaling issues" refers to difficulties and complexities stemming from the applicability of the data measured in the scaled experiments to the conditions expected in the prototype. These issues arise from the impossibility of obtaining transient data from the prototype system under off-nominal conditions. Solving a scaling issue implies developing approaches, procedures, and data suitable for predicting the prototype's performance utilizing scaled models or data [3].

Scale-invariant approaches are ideal for exploring and predicting behaviors in real prototypic applications. Scale invariance represents entities that are independent of scale of length, such as conservation laws and correlations between certain variables. By admitting the scale invariance for conservation law, direct numerical simulation (DNS) that directly solves conservation equations is applicable to scenarios at all scales. And the scale invariance in these correlations needs to be validated in large-scale and integral effect tests (IETs) through scale-distortion analysis. There are two kinds of scale-invariant approaches: (1) a full-scale (or physics-conserved) experiment, which is (presumably) independent of facility scale or (2) DNS modeling, in which local information is solved accurately with very fine mesh. By confirming the validity and consistency of variable correlations in a specific condition across all scales of length, some closure models that accurately describe these correlations can be applicable to scenarios at all scales that satisfy the condition. In NTH, physical models are usually developed in small-scale SETs because full-scale experiments are hard to build while many full-scale tests are required. Meanwhile DNS is a computationally expensive way to deal with the system scenario simulations. Reduced-order models (e.g., large-eddy simulation [LES], Reynolds-averaged Navier-Stokes [RANS] models) and system codes are not scale-invariant approaches. That is why scaling distortion, which refers to any discrepancy between the applied, scaled parameter and the referenced plant parameters, exists in system simulation. Although scaling distortion exists, advanced coarse-mesh computer codes are widely used in NPP safety analyses because of both cost and time effectiveness. The effect of scaling on the model error and the consequent uncertainty calibrated by using data from scaled experiments can greatly influence the accuracy of a simulation, leading to unknown error and uncertainty, called scaling uncertainty. Although very complex scaling methodologies were proposed (some of them – Hierarchical Two-Tiered Scaling (H2TS) [4], Fractional Scaling Analysis (FSA) [5], and Dynamical Systems Scaling (DSA) [6] – are able to quantify these distortions), it is recognized that a complete similarity between the prototype and the model cannot be achieved, particularly in a complex NPP system. Therefore, in V&V procedure of system codes scaling issue has to be addressed, see for example GRS method which includes Code Scaling, Applicability and Uncertainty (CSAU) procedure. [7]

Usage of computational codes—for the evaluation of safety margins, the training of reactor operators, the optimization of the plant design, and the development of emergency operating procedures—is wide and has been growing. At the same time, V&V has been recognized as a mandatory prerequisite of their applications. In 1974, the United States (U.S.) Nuclear Regulatory Commission (NRC) published rules for loss of coolant accident (LOCA) analysis in 10 CFR 50.46 [8] and Appendix K [9]. It established initial licensing procedures with a conservative approach. However, considering the issue of scaling distortion, conservatism proven in reduced-scale tests may become invalid in full-scale plants. As a result, the NRC initiated an effort to develop and demonstrate the BEPU method. This provides nuclear plant operators with more economic gains and less conservatism. The CSAU method was formulated to provide more-realistic estimates on plant safety margins for a large-break LOCA in a pressurized water reactor in 1990 [10]. In 2005, the NRC issued another important contribution, Regulatory Guide 1.203, "Evaluation Model Development and Assessment Process (EMDAP)," a demonstration of a validation framework that is considered acceptable for the best-estimate calculations of NPP transient and accident analysis [11]. Mesh effect on code and model scalability was not fully considered in CSAU and EMDAP. They both recognized the existence of mesh sensitivity and required a mesh-sensitivity study to make sure important figures of merit (e.g., peak cladding temperature) were not significantly impacted. They assumed that a "constant" uncertainty was introduced between the scaled tests and plant application by applying the same modeling guidelines and consistent mesh configurations. However, the fact that mesh size could be one of the key model parameters and would influence code and model applicability was not fully considered because mesh sensitivity was performed before the code-scalability analysis. Although the importance of code-scalability analysis has been well recognized and emphasized in both CSAU and EMDAP, it is difficult to perform with the tight connection between main error sources and error or uncertainty propagation due to scaling uncertainty. Especially in EMDAP Step 19: assess scalability of integrated calculations and data for distortions, necessary techniques that are deficient on data assimilation or scalability assessment. A method is urgently needed to bridge the scale gap and work as a supplement to the implementation of EMDAP considering the industry requirements on validation of evaluation models.

1.3. Issue #3: Insufficient Data Planning

In the most-recent decade, thermal-hydraulic research has produced a large amount of experimental and numerical data which, if measured in petabytes, perhaps is several orders of magnitude more than all accumulated data of the previous history of thermal hydraulics. However, there is still a severe lack of data to validate multiphysics, multiscale capability because very little experimental and plant data are directly relevant to and usable for validation of high-fidelity mechanistic models and codes, particularly when advanced reactor designs are involved. [12] Although remarkably large amounts of data have been generated via experimental tests, only a small portion of data is used for validation and uncertainty quantification (VUQ) of simulation models and codes. For instance, to evaluate the performance of a simulation code on an IET, hundreds of measurement channels are mustered for each new test run of an integral-test facility, but only a few data points are used for assessing and calibrating the simulation code to achieve a successful code-to-data comparison. This situation was defined as “data-rich, knowledge-poor” in [13], which indicates that even if remarkably large amounts of data have been generated, only a very small portion of the data is used for a temporary success of VUQ, but the validated models and codes may be not applicable for other conditions. In other words, data are still not adequate to support a wide range of continuing efforts in calibration and validation of advanced models and codes with the existing modeling and simulation frameworks.

Due to the current data-rich, knowledge-poor situation, the application domain for new reactor designs is not always met by the validation domain, including existing available and relevant validation data, as shown in Figure 1. The inevitable discrepancy between application domain and validation domain leads to a high cost in the designs of experimental and numerical data because of insufficient usage of existing data and insufficient planning on the experimental and numerical data production. Many diverse experimental and high-resolution numerical tests have been performed to satisfy the requirements of data quality and quantity for enlarging validation domain to match application domain.

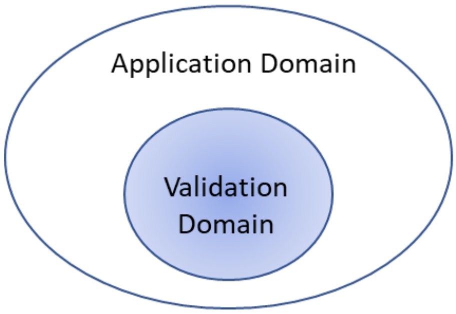

Figure 1. Relationship between validation domain (including existing available and relevant validation data) and application domain (including conditions in new reactor designs).

Therefore, in [13], a question was proposed as “what are fundamental obstacles on the path to efficient use of multi-dimensional, high-resolution data, including physical experimental and numerical simulation data, to reduce a prediction's uncertainty in nuclear reactor thermal hydraulics?" To deal with this question, as first defined in [14], a validation data plan (VDP) is defined as "a dynamic planning instrument to guide and, potentially, optimize activities on data production and acquisition (e.g., through new experiments or plant measurements), data analysis and management (e.g., qualification, classification/meta-data, archiving), and data usage so that they enable effective support for development, assessment, and application of simulation tools intended for a challenge problem." Based on the concept of the VDP, the question has evolved into "how to build a sufficient VDP for a new design?"

2. Opportunities

The enormous progress in science, technology, and engineering in past decades brings opportunities to help deal with these proposed NTH issues. Some capabilities that are enabled in this environment have been summarized in [13], which are still instructive and informative today:

(1) "*Increasing affordability of advanced experimental and diagnostic techniques for the experimentation under some high-temperature high-pressure conditions of interest to reactor applications.*" It provides a technical basis for generating necessary but extreme experimental data for VUQ purpose.

(2) "*Advancement of data science, including statistical analysis methods and tools for processing of multi-field, multi-dimensional heterogeneous datasets, data mining, pattern recognition, data aggregation, and data assimilation.*" Recently, some state-of-the-art machine learning (ML) and statistical tools (e.g., artificial neural networks [ANNs], Gaussian processing regression [GPR]) have been widely applied for different purposes in fluid dynamics that are also of interests in NTH applications. [15, 16, 17]

(3) "*Methods and tools for sensitivity analysis, uncertainty quantification, model calibration and validation, and design of experiments to maximize the data's informative value.*" Based on the concept of Total-Data-Model-Integration (TDMI), a data-driven framework has been proposed for the VUQ of multiphase CFD (MCFD) solver. [18]

(4) "*Advanced methods in computational physics that enable effective and accurate solutions for complex non-linear multi-scale problems.*"

(5) "*Advancement in computer science and software engineering that provide methods and tools to accommodate increasingly and necessarily sophisticated software architectural requirements in a new modeling framework (e.g., flexible data-model integration).*" Some advanced flexible frameworks have been developed for different purposes in data-model integration, such as LOTUS [19] and RAVEN [20].

(6) "*Affordable data storage and computational power needed for data processing, sensitivity and uncertainty analysis, model calibration and time- and space- resolved high-fidelity simulations*."

(7) "*Successes and insights from developments in theory and application of CFD in broad areas outside NTH including MCFD*."

(8) "*Community-wide experience, shared best practice, standards development and accumulative knowledge base from using, innovating, and pushing existing methods and tools in NTH to the limit, particularly driven by common goals in nuclear reactor safety.*"

Particularly, ML-based methods have recently emerged as a valuable approach to aid the development and application of methods for solving modeling and simulation issues in NTH. Some literature reviews have been performed in the companion paper "ML in Nuclear Thermal Hydraulics, Part 1: Fundamentals, Classification, and Recent Advances." There are two main purposes of these applications; one is developing data-driven closure models to replace empirical correlations for specific phenomena such as [21, 22] while the other is developing data-driven surrogate models to directly quantify the simulation uncertainty. [23, 24, 25, 26, 27] These application have constructed very diverse and solid technical bases for improving the use of ML in dealing with the proposed NTH issues. The rapid progress of ML techniques in other industrial fields also provides very valuable lessons to some similar problems. However, due to ML uncertainty, insufficiency of data quality and quantity, and lack of cognition about how to efficiently incorporate knowledge and data, challenges of adapting ML techniques still exist, where some new perspectives and advanced frameworks should be proposed for different purposes in NTH applications.

3. Perspectives

3.1. Perspective #0 (Concept): Local Scale Invariance vs. Global Scale Gap

Over the past few decades, many nuclear reactor designs with different systems, geometries, and powers have been proposed. The respective global characteristics might be an "extrapolation" to previous simulations and experiments, which brings large uncertainty to the demonstration studies using previously developed models (it is worth to mention that most of the experimental data were obtained for water cooled reactors). Relevant thermal-hydraulic experiments with a wide range of scale must be redesigned to validate the applicability of codes and models for these new global conditions. In some conditions, it is possible that local physical parameters or variables in the local cells are similar even when the global characteristics totally changes. Global and local characteristics are differentiated: the former indicates a global or macroscopic state, observation, and deduction of the physical condition, such as the dimension, geometry, structure, boundary condition, and non-dimensional parameters that represent the underlying global characteristics. The latter refers to the microscopic state, observation, and deduction of the physical condition. For example, the global characteristics of turbulent flow can be characterized using Reynold (Re) number. No matter how the Re number or geometry changes, the local characteristics always involve turbulence if the Re number is big enough.

In [25], a concept of physics coverage condition (PCC) was defined to represent the coverage or similarity of existing data/cases and target data/cases by considering both global and local characteristics. Four different physics coverage conditions are defined and classified: global interpolation through local interpolation (GILI), global interpolation through local extrapolation (GILE), global extrapolation through local interpolation (GELI), and global extrapolation through local extrapolation (GELE). For instance, there are several cases for single-phase fully developed flow in a pipe of diameter *D*: local characteristics and values of Re_D representing the global characteristics are listed in Table 1. Assuming some cases as existing data and others as target simulations, four different PCCs can be specified, as shown in Figure 2.

Table 1. Example of different global and local characteristics.

Case	Global Characteristics	Local Characteristics
1	$Re_D = 10^2$	Laminar Flow
2	$Re_D = 2.5 \times 10^3$	Laminar–Turbulent Transition
3	$Re_D = 1 \times 10^4$	Turbulent Flow
4	$Re_D = 2 \times 10^4$	
5	$Re_D = 3 \times 10^4$	

GILE Global Interpolation through Local Extrapolation Case: 1 + 3 → 2	**GELE** Global Extrapolation through Local Extrapolation Case: 1 + 2 → 3
Global Interpolation through Local Interpolation Case: 3 + 5 → 4 **GILI**	Global Extrapolation through Local Interpolation Case: 3 + 4 → 5 **GELI**

Figure 2. Illustration of PCC considering global and local characteristics. [25]

The *GILI condition* represents a situation where both global and local characteristics of the target case (Case 4) are identified as an interpolation of existing cases (Cases 3 and 5). The physics of the target case are globally and locally "covered" by existing cases. The model developed using the data from Case 3 and 5 is reliable to predict Case 4.

For the *GILE condition*, even if the global physical condition of the target case (Case 2) is covered by existing cases (Case 1 and 3), data from existing cases are not able to predict the target case because local characteristics are different. In fact, the models developed from experiments of laminar flow or turbulent flow are not applicable for transition prediction.

GELE condition has the same problem: models developed from the experiments of laminar flow are not applicable for turbulence prediction. In GILE and GELE condition, existing data do not contain instructive information for the target case, so it is useless no matter how much data are used.

GELI condition indicates a situation in which global physical condition of the target case (Case 5) is identified as an extrapolation of existing cases (Case 3 and 4), but local characteristics are similar, as turbulent flow. The values of some representative parameters (e.g., local velocity gradients) are even interpolative in the existing cases. Unlike in GILE or GELE conditions, the local similarity in GELI condition provides feasibility to take benefits from existing data to estimate the target case.

Instead of endlessly evaluating applicable ranges of models and scaling uncertainty, exploring the similarity of local characteristics opens another door to overcome the globally extrapolative problems. For the specific physics of interest (i.e., the specific physical models), local mesh sizes and numerical solvers are treated as an integrated model. Data obtained from this integrated model can be used to construct a library that identifies and stores the local similarities in different global characteristics. This library can be improved as new qualified data become available. Once the library is built, ML algorithms are applied to find the local data pattern and to make predictions for new conditions.

Currently, the grounded-physics coverage condition for analysis and code/model V&V is the GILI condition, in which existing data or experience has the capability to estimate the target case due to both global and local similarities. GELI condition has this potential capability when sufficient data, appropriate physical features, and ML algorithms are available. The extrapolation of global characteristics indicates different global characteristics, such as a set of characteristic non-dimensional parameters, or different initial conditions/boundary conditions (IC/BCs), or different geometries and structures, or dimensions. The interpolation of local characteristics implies two definitions: (1) from the perspective of traditional phenomena decomposition, the existing cases and target case are designed for the local characteristics with similar length and time scales, such as the turbulence example discussed above and (2) from the perspective of data characteristics, the underlying local characteristics of these cases is assumed to be represented by a set of physical features, and a major part of the data of the target case is covered or similar to the data of existing cases. This similarity is dependent on the identification of physical features and on data quality and quantity.

The essence of defining and distinguishing local and global characteristics is to bridge the global scale gap by relying on scale invariance in local data. Local data include all the local variables or parameters that are directly generated or derived from simulations or experiments. The pattern of local data is defined to represent the scale-invariant properties (e.g., distribution, nonlinearity, statistical features) in local data and the scale-invariant correlations among different subsets of local data. For instance, in the case studies performed in [25, 27], a set of local physical features are extracted from local raw data and informed by knowledge of phenomena, numerical methods, and closure applied. These physical features are expected to represent the scale-invariant properties of local data, which are not affected by global characteristics such as global dimensions, IC/BCs, or different geometries and structures. Local pattern recognition is performed to identify the scale-invariant properties of local physical features and their correlations with local simulation errors of quantities of interest (QoIs) via state-of-the-art ML techniques. The identification of physical features integrates information from the physical system of interest, the closure models applied, and the effect of mesh size and established knowledge on scaling analysis. This approach provides a technical basis for a preliminary development of a data-driven scale-invariant-system simulation technology by treating main error sources and scaling uncertainty together. The goal of case studies in [25, 27] is to demonstrate whether the properties of local data represented by local physical features and their correlations with local simulation errors are scale-invariant. Results showed that the proposed data-driven approach called feature-similarity measurement (FSM) has good predictive capability in GELI and GILI conditions with the extrapolations of different global characteristics (e.g., IC/BC, geometry, and dimension). The conceptual exploration and demonstration of local scale invariance provides a promising potential to deal with scaling uncertainty and a technical basis for a preliminary development of a data-driven scale-invariant-system simulation technology by treating main error sources and scaling uncertainty together. This section is also the technical basis for the following three perspectives.

3.2. Perspective #1 (Solution): Efficiency and Accuracy

Compared to system codes using lumped-parameter models, CFD methods have been widely used for solving transport equations of fluid mechanics by using local instantaneous formulations with finer mesh sizes, where small-scale flow features could be captured. While CFD has the potential to accurately predict the flow behavior and reduce the need for dedicated reactor-operational experiments, it suffers from three key challenges for the system-level analysis of NPP behaviors, namely high computational costs, user effects, and limited understanding on error sources of CFD simulation. Since discretizing the temporal and spatial space on a much smaller scale, CFD simulations require many more cells than a STH simulation. One of the most representative examples is DNS method. As a first-principle-based method, DNS directly solves the Navier-Stokes equations without any closure models, thus making it serve as high-fidelity benchmark data, especially in the single-phase study. Productive CFD simulations must be performed on large supercomputers, rather than a multi-core computer. To bypass the computational cost of the fully resolved high Reynolds number case, researchers either conduct separate effect studies with well-controlled flow conditions [28, 29] to develop individual closures, or adopt computational efficient method, such as Eulerian-Lagrangian and Eulerian-Eulerian methods [30, 31].

Still, based on the concepts of TDMI/GELI/FSM and findings in local scale variance, a workflow of applying FSM for computationally efficient CFD prediction was developed in [26], which is modularized in four independent steps as target analysis, feature identification, training database construction, and error prediction. State-of-the-art techniques and algorithms are applied to realize the goals of each step. FSM identifies local physical features based on the system information (e.g., IC/BC, geometry, structure), closure models that contain the information of phenomena of interest and relevant to model error, and local mesh sizes that affect the model error and mesh-induced numerical error. Since the values of physical features are not only determined by mesh sizes but also other physical parameters, the gaps between simulations with different mesh sizes are reduced, which makes it possible to use this well-trained surrogate model to predict the extrapolation of local mesh sizes and use fine-mesh simulation to inform coarse-mesh simulation. Figure 3 displays the workflow of applying FSM for computationally efficient CFD prediction, which is modularized in four independent steps as target analysis, feature identification, training database construction, and error prediction. State-of-the-art techniques and algorithms are applied to realize the goals of each step.

In a word, to achieve a fast-running and acceptable accuracy, relatively coarse grids are utilized for the nodalization of CFD applications. The physics-informed data-driven approach, FSM, can be used to estimate the simulation error of coarse-grid CFD results and correct them to achieve a comparable accuracy as mapped data profiles from high-fidelity data (e.g., fine-grid CFD results using validated closure models, experimental data). More details can be found in [26].

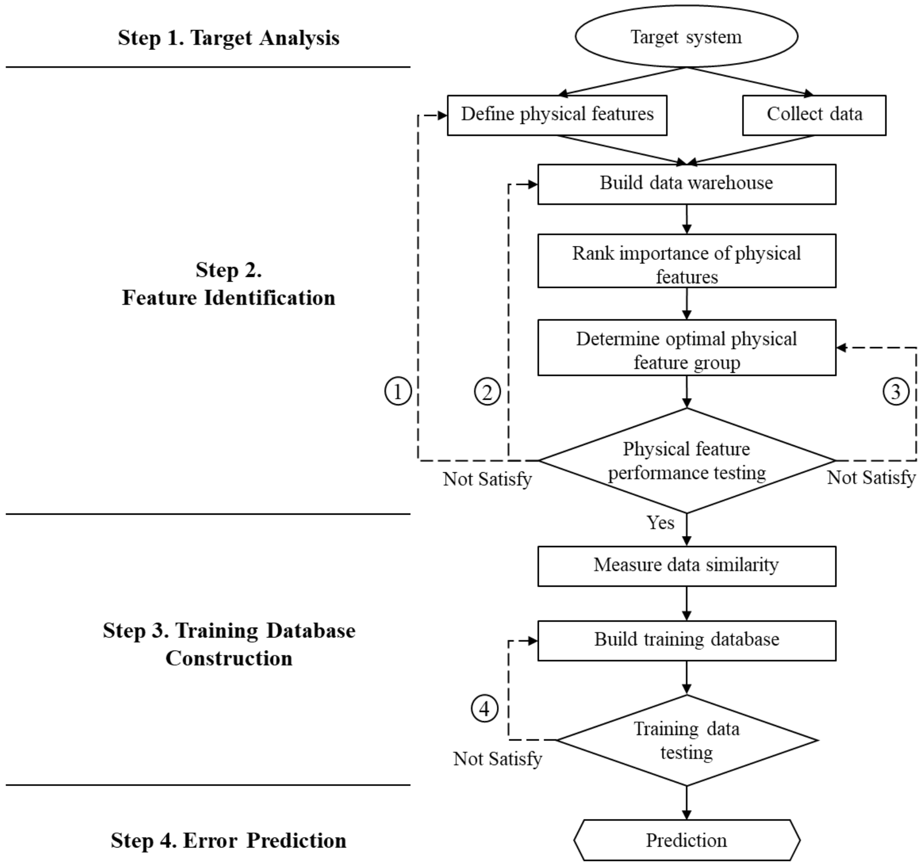

Figure 3. Workflow of applying FSM for computationally efficient CFD prediction. [26]

3.3. Perspective #2 (Potential): Data-driven Scalability Assessment

Evaluation-model adequacy is assessed in Element 4 of EMDAP. Like the scaling approaches applied in Element 2, the assessment process is divided into two parts. The first part (Steps 13–15) focuses on the bottom-up evaluation of closure models and correlations by considering their applicability, fidelity, and scalability. The second part (Steps 16–19) contributes to the top-down evaluation of governing equations, the integrated performance of each code and the integrated performance of the entire evaluation model based on data from IETs. As differentiated from the first part, the second part mainly focuses on the integrated capability and performance of the evaluation model. The first part is clearly described to implement because the target-closure models mostly contribute to a single phenomenon or process. By contrast, the second part is difficult to perform due to the complexity of the involved physics and lack of sufficient validation data. In Step 19, the need to assess the scalability of integrated calculations and data for scaling distortion is proposed; however, it is not clearly explained how to implement this scalability assessment (perhaps each case requires an individual approach). Besides, the importance of nodalization and determination of mesh were not fully considered in the preparation of the calculation input in Step 18. The effect of mesh size on the model/code performance should be fully considered because they also greatly affect both the scalability assessment in Step 19 and uncertainty analysis in Step 20. Furthermore, the extrapolation application of model/code is not mentioned or well guided in the scalability assessment. The classification of different PCCs (GELI/GILI/GELE/GILE) and theoretical exploration on local scale invariance may open a door for these extrapolation conditions.

Based on the concept of TDMI and findings on local scale invariance, a data-driven framework, optimal mesh/model information system (OMIS) is developed to provide simulation error prediction and advice on the selections of optimal mesh size and models for system-level thermal-hydraulic simulation. Relevant details and demonstrations are provided in [24]. The scalability assessment in EMDAP and CSAU is highly heuristic and difficult to implement, and the mesh effect on code/model scalability was not fully considered. Especially in EMDAP Step 19: assess scalability of integrated calculations and data for distortions, a method is urgently needed to bridge the scale gap and work as a supplement to the implementation of EMDAP considering the industry requirements on validation of evaluation models. By treating mesh error, model error, and scaling uncertainty together and introducing ML algorithms to explore the local scale invariance, OMIS framework has the potential to bridge the global scale gap and work as a supplement to the implementation of EMDAP Step 19 in the assessment of integrated scalability, as shown in Figure 4.

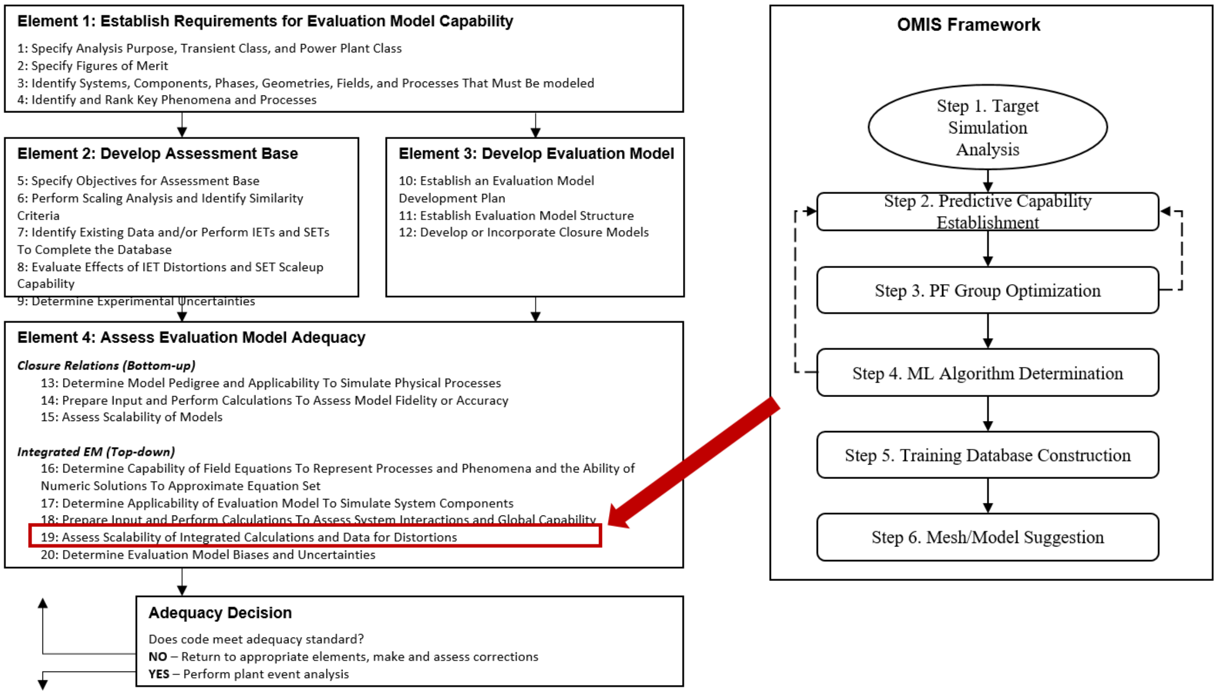

Figure 4. Where OMIS Framework Supplements EMDAP

This section proposes some thoughts on the integration of OMIS framework and EMDAP. As discussed in the previous section, two main drawbacks of EMDAP can be supported and supplemented by OMIS framework: (1) insufficient quantification of mesh effects on model/code scalability and uncertainty analysis and (2) obscure assessment on the scalability of model/code in integrated calculations. The integration, information exchange, and main outcomes between OMIS framework and EMDAP are illustrated in Figure 5. The OMIS framework follows Step 18 of EMDAP, where the input for integrated calculations have been prepared. Then OMIS framework obtains the information from four sources in EMDAP:

- OMIS Step 1 requires identifying the key phenomena, global QoIs, and FoMs that are provided by the PIRT process in EMDAP Element 1.
- OMIS Step 1 requires evaluating the applicability of closure models for the key phenomena in the simulation tool. The model/code information can be provided by EMDAP Element 3, where evaluation model is developed.
- OMIS Step 1 requires input information for integrated calculations, which can be provided by Element 4 Step 18.

- OMIS Step 2 requires collecting high- and low-frequency data, which can be provided by EMDAP Element 2 where database is built.

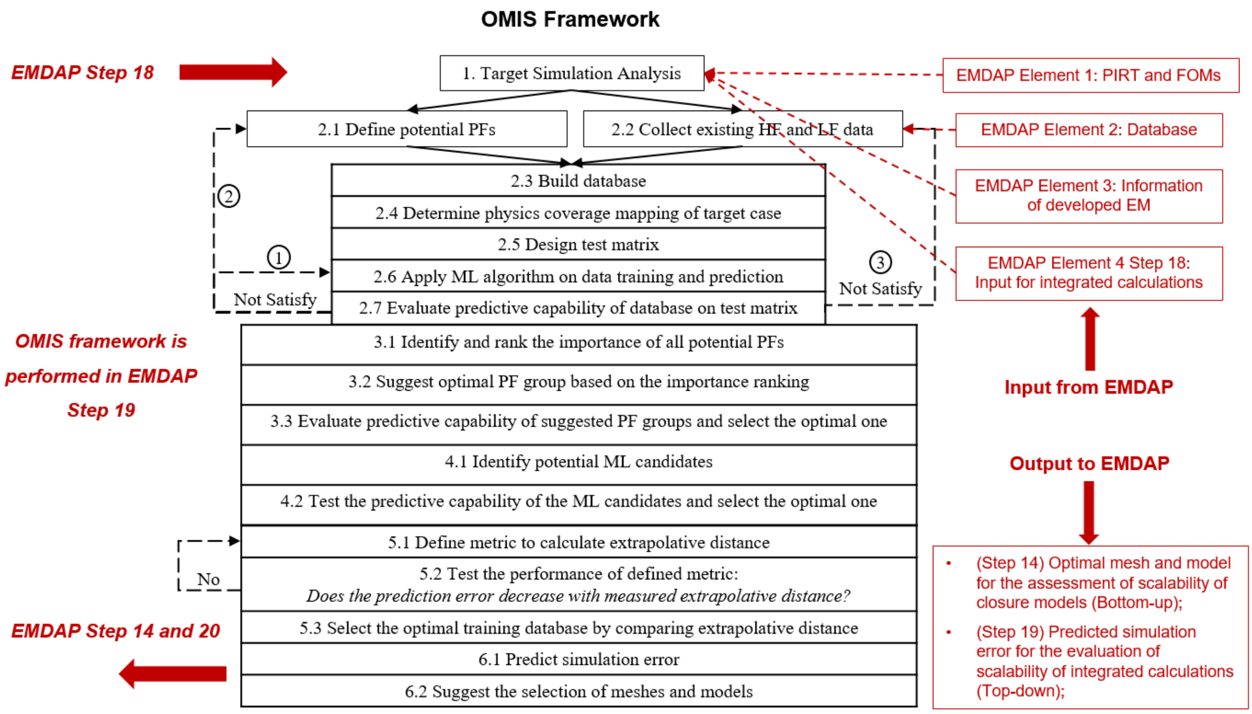

Figure 5. Illustration of the Integration of OMIS Framework and EMDAP (PF: physical feature, HF: high-fidelity, LF: low-fidelity).

The OMIS framework provides three main outcomes back to EMDAP:

- (To EMDAP Step 14) OMIS framework provides suggestion on optimal mesh and model selections. The scalability of these closure models needs to be evaluated using a bottom-up approach, where EMDAP Step 14–15 should be repeated using the suggested mesh.
- (To EMDAP Step 19) OMIS framework provides prediction on the simulation error of QoIs, which can be used to assess the scalability of the model/code in the integrated calculations.
- Besides, the biases and uncertainty in EMDAP Step 20 (determine evaluation model biases and uncertainties) includes model uncertainty/error, mesh error, and other numerical uncertainties with the consideration of scaling effect. This uncertainty has the same content as the concept of simulation error in the OMIS framework.

3.4. Perspective #3 (Insight): Machine-learning-aided Validation Data Planning

Insufficient data planning on data production and usage leads to the formation of the current data-rich, knowledge-poor situation, which also means that the application domain for a new reactor designs is not always met by the validation domain, as shown in Figure 1. The proposal of VDP in [14] gives insight into how to guide and optimize the activities in data production, usage, and management. By leveraging the knowledge on local scale invariance, the capability of VDP has a potential to be significantly improved by exploring the patterns of existing local data. If the concepts of PCCs are applied, the relationship between validation domain and application domain can be defined as shown in Figure 6.

Traditionally, according to the similarity of global characteristics, a major fraction of the validation domain belongs to the GILI condition, the grounded-physics coverage condition for code/model V&V, where the existing data or models have the capability to estimate the target case due to global similarities. Another small fraction of validation domain belongs to GELI condition because the applicability of physical models is very limited for the prediction of extrapolation of global scale, as shown in the left part of Figure 6. For the GILE condition, even if global characteristics of the target case are covered by existing cases, data from existing cases are not able to predict the target case because their patterns of local data are different. For instance, the models developed from experiments of laminar flow or turbulent flow are not applicable for transition prediction, although the global Reynolds number is covered. By contrast, the GELI condition has the potential to be added into the validation domain once the similarity of local characteristics can be well defined and determined. From the perspective of data analysis, the previous validation domain defined by global characteristics may be expanded if it is separated into several new small validation domains reclassified according their different local scale invariance, as illustrated in the right part of Figure 6. Focusing on GELI condition, FSM has a potential to provide insights on the designs of experiments and numerical tests to enlarge the validation domain to reach the required application domain. Another interpretation of Figure 6 is displayed in Figure 7 to illustrate the change from traditional validation domain to machine-learning-guided validation domain.

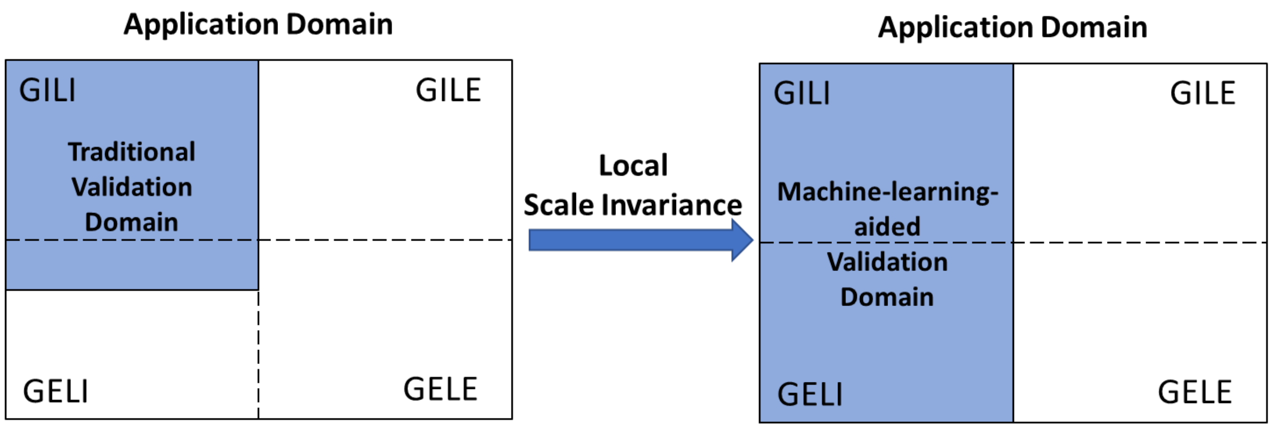

Figure 6. Exploring local scale invariance: a way to reclassify and enlarge the validation domain to reach the application domain.

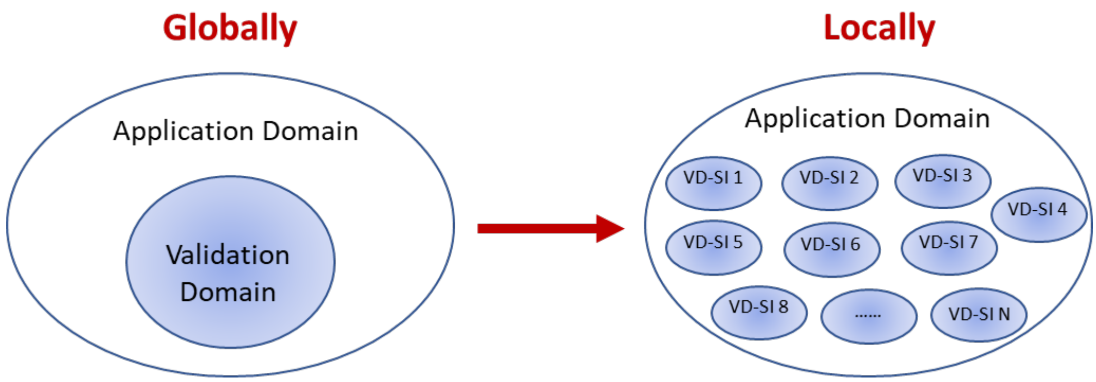

Figure 7. Another interpretation of Figure 6 to illustrate the change from traditional validation domain to machine-learning-guided validation domain. (adapted from [26]). VD-SI means validation domain according to local scale invariance.

The perspective of reclassifying validation domains according to different local scale invariance can be used to efficiently optimize the design of experimental and high-fidelity numerical tests for validation data production, processing, mining, and usage of existing data to effectively support development, assessment, and application of simulation tools intended for a challenge problem. For instance, due to the limited applicability of existing physical models, a large number of experimental tests have to be performed to generate validation data for the uncovered application domain. By applying ML-aided approaches that explore local scale invariance, the simulation error of the models due to scaling uncertainty, model error and mesh-induced error can be estimated to obtain comparably accurate data which can be used to extend the existing validation domain. Costs on the construction of respective experimental facility and test running can be saved or reduced.

4. Conclusions

This paper reviews several technical issues in the field of NTH from three aspects: problems in simultaneously realizing computational efficiency and accuracy of STH modeling and simulation, effects of scaling uncertainty on uncertainty propagation and scalability analysis in transient and accident analysis, and difficulties in optimal data production and usage for the development and assessment of evaluation models. Some opportunities and perspectives of using state-of-the-art machine learning techniques and statistical algorithms are summarized for providing insights in solving these issues. Based on recent demonstration efforts, the conceptual exploration of local scale invariance provides a promising potential to deal with scaling uncertainty and a technical basis for a preliminary development of a data-driven scale-invariant-system simulation technology by treating main error sources and scaling uncertainty together. A framework of realizing computationally efficient CFD predictions for STH simulation was introduced to achieve an optimal balance between efficiency and accuracy. Suggestions and insights are also provided to perform data-driven scalability assessment and machine-learning-aided validation data planning.

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