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Transfer learning for efficient meta-modeling of process simulations

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ABSTRACT

In chemical engineering applications, computational efficient meta-models have been successfully implemented in many instants to surrogate the high-fidelity computational fluid dynamics (CFD) simulators. Nevertheless, substantial simulation efforts are still required to generate representative training data for building meta-models. To solve this problem, in this research work an efficient meta-modeling method is developed based on the concept of transfer learning. First, a base model is built which roughly mimics the CFD simulator. With the help of this model, the feasible operating region of the simulated process is estimated, within which computer experiments are designed. After that, CFD simulations are run at the designed points for data collection. A transfer learning step, which is based on the Bayesian migration technique, is then conducted to build the final meta-model by integrating the information of the base model with the simulation data. Because of the incorporation of the base model, only a small number of simulation points are needed in meta-model training.

1. Introduction

Computational fluid dynamics (CFD) is a powerful tool for analyzing fluid flow and transport phenomena. Its implementation to the chemical processes has been widely researched and many successful applications (Chen and Tan, 2012; Chuang and Chen, 2014; Pan et al., 2016) were reported in the past decade. A notable advantage of CFD is its capability of high-fidelity modeling of complex chemical processes involving multi-phase flows, mixing of fluids, heterogeneous reactions, intricate reactor geometry, etc. Such high-fidelity CFD models generally require a large number of ordinary differential equations (ODEs) and partial differential equations (PDEs) to characterize various physical factors and spatial-temporal variations of the system. Substantial computational resources and time (hours to days) are needed for even one simulation. Hence the simulation study becomes a long and arduous task if it has to be performed many times for some specific applications, e.g., sensitivity analysis (Kajero et al., 2017a; Razavi et al., 2012), model calibration (Kajero et al., 2016), consequence analysis (Loy et al., 2017) and optimization (Chen et al., 2014; Chuang et al., 2016; Manfren et al., 2013; Boukouvala and Ierapetritou, 2014).

Recently, meta-modeling has been introduced as a useful methodology to reduce the computation demand of CFD simulations (Wang and Shan, 2006; Wang et al., 2014; Jia et al., 2016; Jiang et al., 2017; Klingenberger et al., 2017). The main purpose of meta-modeling is to use a number of computer simulation data to develop surrogate models (models of model, or meta-models) that predict the system input–output relationship with very little computational cost. There have been already many developments and investigations on meta-modeling, and a comprehensive review of meta-model representation, construction and evolution can be found in a recent survey (Kajero et al., 2017b). In general, the predictive performance of meta-models depends on the choice of how the computer simulations are designed (i.e. design of experiments, DoE) and what types of meta-models are adopted. If the training data are sufficiently representative of the input space and the meta-model is flexible enough to capture input–output relationships, the meta-model developed can be an accurate surrogate of CFD simulations.

Nevertheless, to build meta-models, substantial simulation efforts are inevitably required to generate representative training data. To address this problem, the concept of transfer learning (Pan and Yang,

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2010; Weiss et al., 2016; Tsung et al., 2017) is adopted here to develop meta-models with a reduced amount of simulation data. Specifically, the technique of Bayesian model migration (Yan et al., 2011), which belongs to the family of parameter-based transfer learning, is employed. Model migration is an evolutionary approach that allows us to leverage knowledge learned from a previous process (cast in the form of a base model) in the model development of a new but "similar" process being investigated. Lu and Gao (2008) and Lu et al. (2009) recognized this problem and revealed that model migration is efficient to reduce data requirement for new process model construction. It should be pointed out that process similarity does exist in many problems in chemical process engineering such as scale-up, product grade change for various customers with slightly different specifications, etc. Although the results are quite good, the aforementioned migration studies do not reveal how such similarity helps in model building or whether a migration from a base model dissimilar to the investigated process is detrimental. In addition, in previous research, the model migration technique has seldom been utilized for meta-modeling of CFD simulations.

Furthermore, many real-world engineering problems consist of explicit constraints on the system inputs and implicit constraints on system outputs. The explicit constraints define the search space, which can be addressed with existing DoE methods. However, it is unclear how implicit constraints should be handled. For example, in an exothermic reaction system, the pressure, inlet/outlet flow rate, inlet reactant concentration, and cooling system are manipulated to maximize the reactant conversion as well as preventing the thermal runaway. If an improper operation condition was implemented to CFD simulations, the runaway situation may cause numerical errors, and even if the simulation converges the results are not very useful in terms of learning response surface in the feasible region. The challenge is thus how to generate initial experiments that are as feasible as possible over the complete domain of interest while minimizing the simulation cost. So far, to the best of our knowledge, there has been no work that addresses meta-model construction for high-fidelity CFD model with implicit constraints.

In this paper, a base model and a Bayesian migration scheme are integrated for efficient meta-modeling of complex chemical process simulations, where the base model is a computationally efficient model describing a specific problem that is similar to the high-fidelity CFD one being studied. Generally, such a base model can be obtained from an existing well-studied model or be developed by fundamental theories. The aim of using the base model is to give a fast and rough prediction of the high-fidelity CFD simulations and at the same time use its feasibility information to assist the computer DoE. In addition, the proposed Bayesian migration scheme implements a functional scale-bias correction to merge the base model into a flexible Gaussian process regression (GPR) meta-model and applies Bayesian inference with the computer DoE data for meta-model training. Expectedly, the quality of the base model, as measured by its similarity to the high-fidelity CFD model, will have a significant impact on the number of computer experiments (i.e. expensive CFD simulations) required for reliable meta-model development. This has been explored by using base models that encode the "right" or "wrong" physical mechanisms, and a base model that does not rely on any physical mechanism. The results show that, as expected, a base model with a good physical basis is beneficial to meta-modelling. It is also assuring that even if a wrong physical base model is used, the resulting meta-model is no worse than when no physics is used (i.e. the model purely based on the computer experimental data). In other words, no negative transfer is observed in the case studies. Finally, it appears that the correct identification of the search space and the process constraints is at least as important as the absolute accuracy of the base model. These observations will be elaborated and discussed subsequently.

The remainder of this paper is organized as follows. In Section 2, the transfer learning based meta-modeling scheme is introduced in detail. Subsequently, a complex CFD model of a non-isothermal continuous stirred tank reactor (CSTR) is described in Section 3, together with several base models with various forms. In Section 4, the effects of choosing different base models in model migration are studied. In addition, a comparative study is conducted by comparing the results of migration and a conventional meta-modeling approach. Finally, Section 5 concludes the paper with remarks.

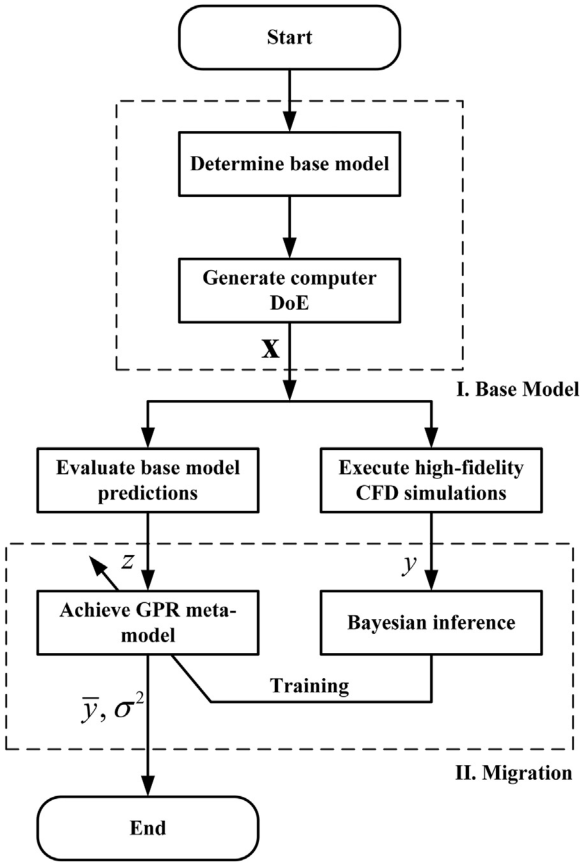

Fig. 1 – The flowchart of the proposed meta-modeling approach.

2. Methodology

Fig. 1 depicts the overall flowchart of the transfer learning based meta-modeling strategy which integrates two specific parts, i.e., base model setup and model migration. The base model is used to roughly mimic the input-output relationship of the high-fidelity CFD simulations as well as help to design the computer experiments. The model migration step incorporates the base model in a flexible GPR structure and applies Bayesian inference to obtain the final meta-model from the CFD experimental results.

The key advantage of the proposed strategy is that, as long as there is sufficient similarity between the base model and the CFD model, only a small number of CFD simulations are required to build a meta-model with high accuracy. In other words, the computational time to run the CFD experiments is largely reduced. The entire procedure and the details of different steps are presented in the following subsections, whereas the effects of the quality of the base model are discussed in Section 3.

2.1. *Generation of base model*

Generation of the base model is an important start to the proposed meta-modeling strategy especially for the CFD problems with implicit constraints. As mentioned above, the target of the base model is to give fast and rough predictions of the CFD simulator and at the same time use its feasibility infor-