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Surrogate modelling and uncertainty quantification for multiscale simulation

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Publication date
2022

Link to publication

Citation for published version (APA):
Ye, D. (2022). *Surrogate modelling and uncertainty quantification for multiscale simulation*. [Thesis, fully internal, Universiteit van Amsterdam].

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Download date:29 Sep 2023

Chapter 6

Conclusions and outlooks

This PhD thesis is inspired by the need for UQ for the multiscale ISR model and focuses on UQ and sensitivity analysis of ISR model uncertain parameters as well as the surrogate modelling techniques applied to improve the computational efficiency of model evaluation in both non-intrusive and semi-intrusive UQ.

Chapter two presents a detailed comparison between semi-intrusive UQ and non-intrusive UQ approaches with surrogate modelling techniques based on the ISR2D model. The results show that both semi-intrusive and non-intrusive are valid and efficient methods to perform UQ, but have their own advantages and disadvantages in terms of accuracy of UQ estimation, speedup and granularity. The result offers a guide to choosing between two UQ methods for multiscale simulations.

In chapter three, UQ and sensitivity analysis of the ISR3D model were performed to study the four important uncertain parameters of the model. A GP surrogate model with POD was developed to reduce the computational cost of model evaluation. The UQ and sensitivity analysis demonstrate the significance of each uncertain parameter over the post-stenting recovery and provide a reference for further UQ experiment design of the ISR3D model.

The work of Chapter four was motivated by the need to reduce the high computational cost of 3D blood flow simulation owning to the cyclic structure of ISR3D. The proposed surrogate model combines the surface registration techniques and the reduced-order method together to overcome the issues, including the parametrisation of irregular shapes of domains and the construction of reduced order bases on a reference domain. The accuracy and computational efficiency of the surrogate model were demonstrated based on two numerical examples.

Chapter five introduces a series of UQ patterns (UQPs) for efficient UQ of multiscale models, and categorises them by the level of intrusiveness and optimisation method. Their implementations through the coupling toolkit MUSLCE3 are demonstrated. These UQPs provide the basic building blocks to create tailored UQ for multiscale models.

In this thesis, UQ and sensitivity analysis of the ISR3D model for multiple uncertain parameters have been performed and studied. These parameters are mostly biological parameters, such as the rate of re-endothelialization or the percentage of fenestration in the internal elastic lamina which help us to understand the ISR process. UQ can be further applied to guide the design of stents and their deployment processes. By quantifying the uncertainties of related mechanical parameters such as the shape and thickness of struts, stent deployment depth or material of the stent, the design optimisation problem can benefit from UQ and sensitivity analysis to specify the regime in the parameter space that optimally minimises neointima growth.

Semi-intrusive UQ methods provide an alternative way to construct UQ data for statistical analysis compared to non-intrusive UQ methods. The surrogate model in both cases will inevitably introduce errors into uncertainty estimation. A multi-fidelity method [12, 182] can be applied here for uncertainty analysis as both methods require to evaluate a certain amount of the original model to generate training data. Therefore a multi-fidelity framework can combine both high fidelity data (training data) and low fidelity approximations (generated by or with a surrogate model) together to further improve the accuracy of uncertainty estimation. This method has been used in non-intrusive UQ analysis, but has not been applied to semi-intrusive UQ methods yet. It would be helpful to include the method for further work.

The application of surrogate modelling techniques is mainly driven by the needs of UQ. However other scenarios in biomedical engineering such as real-time simulation [183] also heavily rely on surrogate modelling. In clinical practice, a light-weighted and reliable CFD model can support surgery and clinical decision-making if a real-time prediction of hemodynamics based on patient-specific data is available. The reduced-order modelling framework introduced in Chapter four is split into online and offline processes, which makes real-time prediction possible. By collecting, classifying and constructing a corresponding database of vessel segments or a specific organ in the offline stages, one would be able to perform a real-time simulation based on the framework of the reduced bases.

The construction of the surrogate model in this thesis is mainly based on data-driven methods, including non-intrusive reduced-order modelling, Gaussian process regression and convolution neural network. These methods are light-weighted in prediction but the accuracy of predictions heavily relies on the training data and may fail when dealing with extrapolation, while the traditional numerical models are physics-based and not limited to any data. How to embed and combine the physics laws as much as possible into a data-driven method is one of the state-of-the-art topics of surrogate modelling.