Non-medical projects

Assessment of uncertainty in CALPHAD predictions for Molten Salt Reactor fuel (BEP)

Understanding and predicting nuclear fuel behaviour in innovative type of reactors, such as the Molten Salt Reactor, is a key step for their future development and deployment. The CALPHAD (CALculation of PHAse Diagrams) method is a proven and indispensable tool in this endeavour and it is currently used to generate customized thermodynamic databases. Based on the developed models, thermochemical equilibrium calculations are performed allowing the prediction of the thermodynamic properties and the evaluation of the safety margins for the potential fuel mixtures.

For reactor designer and regulatory bodies, knowledge of the uncertainty associated with the results from CALPHAD is crucial. Currently however, the reliability of these predictions is only inferred by comparing the calculated results to experimental phase equilibria data, resulting in a region of confidence which is limited to known composition and temperature regimes. Rigorous, comprehensive evaluation of uncertainties is lacking. At the same time there is substantial knowledge about uncertainty propagation and evaluation methods applicable to generic computational problems. The goal of this project is to make the first step towards the accurate and computationally affordable prediction of uncertainties in CALPHAD calculations by using and adapting advanced uncertainty quantification methods.

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Multi-fidelity adjoint-aided Polynomial Chaos Expansion for uncertainty quantification of multi-physics problems (MEP)

Almost all modern engineering problems include complex, multi-scale, multi-physics simulations, taking into account different phenomena in the investigated system, typically by coupling together several different code systems separately modelling physical, chemical, mechanical, etc. interactions. Such models both involve a very large number of parameters (such as geometrical sizes, material properties, modelling assumptions), as well as significant non-linearities due to the complicated interaction between the different phenomena. For accurate predictions, it is essential to correctly analyse how unavoidable uncertainties in the input parameters effect the calculated quantities of interest.

Polynomial Chaos Expansion methods provide an attractive solution to this problem by building a meta-model from multivariate polynomials of the uncertain inputs. Since the method relies on running the complex multi-physics model for different realization of the inputs, its computational cost scales with that of the original model. Using multi-fidelity approaches, i.e. a sequence of models, starting with low-fidelity, simple but fast solutions to the problem with limited accuracy, through mid- to high-fidelity solutions on fine grids, with all physics interactions taken into account, being computationally expensive but highly accurate can provide a solution to the problem. In such approaches, we use many cheap, low-fidelity model calculations to get most of the model behaviour, and rely on only a few expensive high fidelity runs as corrections to increase accuracy. Moreover, when adjoint capabilities are available in either only the low or both the low- and high-fidelity models we can use the additional derivative information to speed up the meta-model construction. This project will focus on the research, implementation, testing and large scale application of such frameworks.

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Efficient design of experiment for high dimensional stochastic multi-physics problems (MEP)

Truly high dimensional engineering problems, involving hundreds or thousands of parameters are one of the most important outstanding challenges in computational physics. Such models are typically complex, multi-scale and multi-physics calculations, where a single run can take hours, days or even weeks on a modern cluster. Thus, extensive sampling in such cases – needed in traditional uncertainty analysis – is clearly infeasible, which makes meta-modelling approaches highly attractive for these applications. Still, the so called "curse of dimensionality", i.e. the exponentially increasing number of model runs needed with the increasing number of parameters is an unavoidable challenge, making research into computationally efficient solutions of high priority.

In this research, design of experiment approaches will be studied to tackle the high dimensionality of the problem. These approaches rely on grouping together different input parameters and handling them together to infer the importance of the whole group. By randomly group parameters in different runs, the expectation is that inputs always being in an "important" group are themselves important, thus the individual effects can be inferred from repeated group wise parameter perturbations. We will study both random and systematic grouping and refining approaches to design effective algorithms.

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Proposal for internship at NRG (Arnhem)

Reactor core design

September 7, 2020

I. GENERAL CONTEXT

The core design of a nuclear reactor is a challenging task due to the theoretically infinite number of possible fuel loading patterns. NRG's software ROSA (Reloading Optimization by Simulated Annealing) is successfully being used for in-core fuel management of more than twenty-five Pressurized Water Reactors (PWRs) across the world. ROSA combines a 3-D neutronics and thermal-hydraulic core simulator with a simulated-annealing optimization algorithm, which searches for an optimal loading pattern by means of a stochastic approach. The code can evaluate up to billions of core design options in a day, based on any combination of more than sixty optimization parameters. These range from safety operational margins to energy production and fuel cost saving. Since a whole-core coupled depletion calculation must be performed for each candidate loading pattern, computing speed is one of the essential requirements for ROSA. For this reason, its neutronics solver is based on the kernel method, a particularly fast type of nodal method in which assembly-size nodes are coupled via neutron interaction probabilities computed under a number of simplifying assumptions.

II. GOAL OF THE INTERNSHIP AND RANGE OF TOPICS

A version of ROSA is currently being developed for Boiling Water Reactor (BWR) core design. Compared to PWRs (for which the robustness of the kernel method has been extensively tested), this type of reactor has a significantly higher core heterogeneity, due to strong coolant density variations, more heterogeneous fuel composition, and long-lasting insertion of control blades for power shaping. These features may invalidate or weaken some of the assumptions underpinning the kernel approach used in ROSA.

In the framework of the ROSA BWR version development, the internship will be focused on one of the following topics (depending on the interest of the applicant):

- an assessment of the impact of the approximations adopted in ROSA's neutronics solver on the solution of the optimization problem for BWR core design;
- the implementation of more accurate BWR core physics models (for example, modeling of spectral history effects);
- the development of a method for control-blade pattern optimization;
- the extension of the code with new optimization parameters and additional functionality.

III. TEAM AND OFFER

The internship will take place in the Fuel Management Services unit of the C&S (Consultancy and Services) department of NRG in Arnhem (the Netherlands). The student will be working side by side with ROSA's developers. High flexibility is ensured for the time frame and duration of the internship. Working remotely is possible, with a minimum number of days (one or two) to be spent in the office.

The student will receive a reimbursement of expenses (400€ gross per month) and a travel allowance. An additional compensation of 200€ net per month can be claimed for housing if the student temporarily needs to relocate.

IV. CONTACT

The interested student is welcomed to contact Pieter Wakker (e-mail address: **wakker@nrg.eu**).