Uppsala University is a comprehensive research-intensive university with a strong international standing. Our ultimate goal is to conduct education and research of the highest quality and relevance to make a long-term difference in society. Our most important assets are all the individuals whose curiosity and dedication make Uppsala University one of Sweden’s most exciting workplaces. Uppsala University has over 45,000 students, more than 7,000 employees and a turnover of around SEK 7 billion.

The Centre for Interdisciplinary Mathematics (CIM) at Uppsala University conducts interdisciplinary research connecting the mathematical sciences and other areas of science and industry. CIM offers training and expertise in mathematical modelling and computer simulation, and hosts a Graduate school since 2011; for more details see CIM’s website. We are now looking for up to four PhD students who will join CIM’s Graduate school and work on proposed research projects. All available projects can be found on the project webpage. The Nuclear Data specific project is also listed below.

**Duties:** A PhD student should mainly focus on her/his own graduate education, which comprises four years of study. The position can also include other departmental duties (up to 20%), in which case the position is extended accordingly. The PhD student will work with an interdisciplinary research project, with at least two advisers representing different scientific areas, or one from a company or a research institute and one from academia.

The PhD students are expected to engage actively in the activities of the centre, such as seminars and workshops. They will be required to take at least 30 hp (6 months full time study) PhD courses in mathematics, modelling, statistics, scientific computing, offered by e.g. Department of Mathematics and Department of Information Technology.

**Requirements:** The candidates are expected to have an interest in applied mathematics and/or developing models in an interdisciplinary context. A PhD student position requires a master’s degree in a field that is relevant for conducting research in applied mathematics, e.g., mathematics, engineering physics or scientific computing. Candidates with a
Machine learning regression for large scale nuclear physics and engineering.

background in another area of science, e.g. chemistry or biology, with a strong competence and interest in mathematical modelling are also encouraged to apply.

Application: The application should include a personal letter (of max 1 page) containing applicant’s reflection on the selected research project (among the proposed ones), with focus on a personal motivation for selecting the project, and arguments why the applicant’s background fits the selected research topic. The application should also include a Curriculum Vitae (CV), copies of diplomas and certificates, a copy of master’s degree dissertation if available (alternatively, or in addition, other written scholarly works/articles can be included).

Acceptance as a PhD student within the Centre for Interdisciplinary Mathematics will be subject to the condition of acceptance by an appropriate Uppsala University department into a PhD research programme. The successful candidates may start in September 2021 or according to agreement.

Rules governing PhD students are set out in the Higher Education Ordinance chapter 5, §§ 1-7.

The application must include:

1. The names of the intended advisers and the project title
2. A personal letter of maximum one page (see above)
3. Curriculum Vitae (maximum two pages)
4. A copy of degree diploma (if degree is completed) along with a transcript of grades
5. List of publications (if any)
6. A copy of master’s thesis or a draft and a detailed time plan for the rest of the work if it is not yet completed. The applicant must have a complete master’s degree before the starting date of the PhD position
7. Name, position, relation to the applicant and e-mail addresses of two reference persons
8. Other documents that the applicant wants to be considered in the evaluation

Salary: According to local agreement for PhD students.

Starting date: September 2021, or as otherwise agreed.
Type of employment: Temporary position according to the Higher Education Ordinance chapter 5 § 7.

Scope of employment: 100 %.

For further information about the project please contact: Henrik Sjöstrand, Henrik.sjostrand@physics.uu.se

Please submit your application by 31 March 2021, UFV-PA 2021/616.

Are you considering moving to Sweden to work at Uppsala University? Find out more about what it’s like to work and live in Sweden.

More information about the position can be found here.

Submit your application through Uppsala University's recruitment system here.

Project description - Machine learning regression for large scale nuclear physics and engineering

Uncertainty quantification (UQ) in modeling combines two challenging tasks: scientific modeling and application of advanced statistical methods. UQ is particularly important in nuclear physics and engineering, where uncertainties of fundamental quantities can affect important safety parameters. Applications of nuclear physics modeling range from fusion and fission reactors, medical treatment, electronics, space physics, stellar nucleosynthesis, and accelerators, and require high fidelity knowledge of the underlying process that describes the nuclear interactions.

This project concerns the development of novel methods in the field of nuclear modeling and Nuclear Data (ND) UQ in the realm of nuclear engineering. The ND UQ methods, nuclear physics models, and ND libraries will be improved by including methods from the machine learning community, e.g., hierarchical Bayesian models, Bayesian non-parametric models based on Gaussian processes (GP), and sparse methods. This allows us to incorporate statistically well-founded, reliable, and quantitative methods for the use of calibration data. More specifically, the combination of such methods will enable us to handle the misspecifications of nuclear models and problems with experimental data in an automated and robust way. The application of sparse approximations enables the application of the new methods on a large scale, which is a requirement to deal with the large amount of experimental data and data produced in simulations. With the new methods, we will go beyond the state-of-the-art for ND UQ for nuclear engineering as well as increasing our nuclear physics knowledge.
Machine learning regression for large scale nuclear physics and engineering.

**Specific goals**
1. Improve methods to include discrepant and correlated experimental data in UQ methods by, e.g., using hierarchical Bayesian models such as maximum likelihood optimization.
2. Incorporate new approaches such as stage-wise adaptive importance sampling and Bayesian nonparametric methods based on GP, into the field of ND evaluation.
3. Incorporate findings in the main nuclear libraries, such as JEFF and TENDL.
4. Apply the newly developed UQ methods to criticality studies for nuclear reactors.

**State-of-the-art: Total Monte Carlo- linking fundamental nuclear physics to nuclear engineering applications**

Fundamental nuclear physics, and hence nuclear modeling, is essential for the prediction of nuclear reactions. The theoretical framework describing this consists of the optical model; the compound nucleus model; the direct and pre-equilibrium reaction model; fission; \( r \)-matrix theory; and nuclear structure information \[Kon19\]. Combining this framework with millions of data points has allowed the scientific community to ensemble large databases/libraries with ND. These are referred to as Evaluated Nuclear Data Files (ENDFs), e.g., the Joint Evaluated Fission and Fusion File (JEFF) and the Talys Evaluated Nuclear Data Library TENDL \[Kon19\]. This data consists of different quantities, such as cross-sections, angular distributions, fission yields, neutron emission, and single and double differential data. However, the experimental data is incomplete and associated with uncertainties and inconsistencies. Furthermore, the nuclear theory is only approximative and contains both uncertainties and model defects. Consequently, the ND is associated with uncertainties and it has since long been recognized that the estimation and propagation of uncertainties are paramount in the design and development of future nuclear applications \[WPEC-26\]. Today, ND libraries do not include complete covariance information, and many reactor codes do not request uncertainties in the nuclear data input. Thus, the macroscopic output from these codes (flux, energy deposition, reaction rates, dose, criticality, etc.) has unknown uncertainties. Considering the importance of results from reactor codes in developing new reactor concepts and analyze safety margins, this lack of quality assurance is far from satisfactory, with even some safety implications.

**Project Description**

**Construct modeling methods for correlated and discrepant experimental data and correlated integral data**

One of the greatest challenges is to calibrate against experimental data where the covariance information is incomplete, wrong or inconsistent. This is often handled by expert judgment \[Hel17b\], but the results can be biased towards preconceptions of the expert, and this method can be difficult to apply when there is a large amount of data. Another option is to use rule-based approaches such as presented in \[Hel17a\] where a set of rules are constructed to modify the covariance information of the experiments giving the information reported by the experimentalist. This method has the advantage to be transparent, but the results are very sensitive to the choice of rules. Finally, some data-driven methods such as maximum likelihood optimization (MLO) \[Sch17a, Sjo19\] can be used to infer the most likely set of covariances. In the project we will continue to develop hierarchical Bayesian models and their approximative solution via optimization and also investigate the feasibility of other inference methods based on sampling, such as Gibbs sampling and slice sampling, for ND evaluation. In addition, different techniques for marginalization over the likelihood space, will be tested.

**Evaluation and incorporation of new calibration methods into the nuclear data evaluation field**

The EXFOR experimental database comprises roughly sixteen million data points. The models describing the underlying physics for the 2800 isotopes need to be calibrated against this large experimental data set. The complexity of the multi-channel, multi-parameter nuclear models makes such calibration particular challenging. We intend to build on the advances connected to the development of machine learning and applied mathematics to establish new sets of calibration rules.
for nuclear modeling. By using the full-scale experimental information and complete nuclear modeling in combination with different learning algorithms, this could dramatically improve ND modeling, as well as provide the applied community with more meaningful nuclear data. In particular, an extension of the recently proposed Adaptive Monte Carlo [Sch16a] scheme may be more efficient than the currently adopted Bayesian Monte Carlo method [Kon15]. Further, model defects need to be treated and can be treated with GP. A GP creates a set of multivariate random variables from a chosen covariance function [Hel17c] where the choice of the covariance function [Hel17c, Sch19] affects the outcome of the result. In the project we will test different approaches to optimize the co-variance function, both by allowing the hyper parameters to become functional valuers and by testing if a marginalizing the GP Hyperparameters using Sequential Monte Carlo would yield more well-founded uncertainties. We will try to model the model defect in the observable and in the model space simultaneously to obtain increased flexibility in the model. The results will be integrated into new nuclear data libraries and tested in criticality safety and decay heat studies.

Research environment and cross-disciplinary
The project will be co-funded by SKC (Swedish Nuclear Center), which consist of Westinghouse, Swedish Safety Authority and the Swedish nuclear power plant operators. Including these partners into the project will make it possible to disseminate the results within the Swedish “Nuclear engineering Society”. The project will also be tightly coupled to ongoing work at IAEA, the JEFF nuclear data project, and in the OECD / NEA evaluation collaboration. In all these organizations, the treatment of model-defect has been identified to be paramount. In addition, the project will be be carried out in collaboration with PSI, Switzerland, where extensive experience of nuclear data evaluation and nuclear data in application has been built up over the last decades.

As described above, the project will be based on a set of different techniques developed in the machine learning community. Foremost, the goal is to bring in the state of the art of ML to this application. In addition, since nuclear data evaluation problems contain features of particle interest, such as strong long-range correlations, it can pose quite unique challenges to the ML-algorithms to be tested. In such, the project will bring benefits to both the physics, engineering, and mathematics, community. The project will be hosted at the Physics and Astronomy department. Henrik Sjöstrand, with expertise from nuclear data evaluation and nuclear engineering, from Physics and Astronomy, division of Applied Nuclear Physics will be the main supervisor. Rolf Larsson, professor at the Department of Mathematics, with a broad expertise in Mathematical Statistics, will act as co-supervisor. Dimitri Rochman (http://scholar.google.ch/citations?user=IFM4N5UAAAAJ) from PSI, Switzerland, with extensive experience in nuclear data evaluation and nuclear data in applications will also act as co-supervisor.

References
[Hel17a] P.Helgesson, H. Sjöstrand et al., Progress in nuclear energy, 96 (2017)
[WPEC-26] M. Salvatores, NEA/WPEC-26, Uncertainty and target accuracy assessment for innovative systems using recent covariance data evaluations

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